Technical Report

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Characterization and Evaluation of Sites for Deep Geological Disposal of Radioactive Waste in Fractured Rocks

Proceedings from The 3rd ÄSPÖ International Seminar Oskarshamn, June 10–12, 1998

Svensk Kärnbränslehantering AB

September 1998

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Swedish Nuclear Fuel and Waste Management Co Box 5864 SE-102 40 Stockholm Sweden Tel 08-459 84 00 +46 8 459 84 00 Fax 08-661 57 19 +46 8 661 57 19



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Preface

The 3rd Äspö International Seminar was organised by SKB to assess the state of the art in characterisation and evaluation of sites for deep geological disposal of radioactive waste in fractured rocks. Site characterisation and evaluation are important elements for determining the site suitability and long-term safety of a geological repository for radioactive waste disposal. Characterisation work also provides vital information for the design of the underground facility and the engineered barrier system that will contain the waste.

The aim of the seminar was to provide a comprehensive assessment of the current know-how on this topic based on world-wide experience from more than 20 years of characterisation and evaluation work.

The seminar, which was held at the Aspö Hard Rock Laboratory on June 8-10, 1998, was attended by 72 scientists from 10 different countries. The program was divided into four sessions of which two were run in parallel. A total of 38 oral and 5 poster presentations were given at the seminar. The presentations gave a comprehensive summary of recently completed and current work on site characterisation, modelling and application in performance assessments. The results presented at the seminar generally show that significant progress has been made in this field during the last decade. New characterisation techniques have become available, strategies for site investigations have developed further, and model concepts and codes have reached new levels of refinement. Data obtained from site characterisation have also successfully been applied in several site specific performance assessments. The seminar clearly showed that there is a solid scientific basis for assessing the suitability of sites for actual repositories based on currently available site characterisation technology and modelling capabilities.

Olle Olsson Director Äspö Hard Rock Laboratory Swedish Nuclear Fuel and Waste Management Co.

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Session 1

Integrated characterization of potential repository sites and URLs

CHARACTERIZING FRACTURED PLUTONIC ROCKS OF THE CANADIAN SHIELD FOR DEEP GEOLOGICAL DISPOSAL OF CANADA'S RADIOACTIVE WASTES

G.S. Lodha, C.C. Davison, M. Gascoyne

Atomic Energy of Canada Limited, Whiteshell Laboratories, Pinawa, Manitoba R0E 1L0 1998

Abstract

Since 1978 AECL has been investigating plutonic rocks of the Canadian Shield as a potential medium for the disposal of Canada's nuclear fuel waste. During the last two years this study has been continued as part of Ontario Hydro's used fuel disposal program. Methods have been developed for characterizing the geotechnical conditions at the regional scale (500 to 1000 km²) of the Canadian Shield as well as for characterizing conditions at the site scale (~25 km²) and the very near-field scale needed for locating and designing disposal vault rooms and waste emplacement areas. The Whiteshell Research Area (WRA) and the Underground Research Laboratory (URL) in southeastern Manitoba have been extensively used to develop and demonstrate the different scales of characterization methods.

At the regional scale, airborne magnetic and electromagnetic surveys combined with LANDSAT 5 and surface gravity survey data have been helpful in identifying boundaries of the plutonic rocks, overburden thicknesses, major lineaments that might be geological structures, lithological contacts and depths of the batholiths. Surface geological mapping of exposed rock outcrops, combined with surface VLF/EM, radar and seismic reflection surveys were useful in identifying the orientation and depth continuity of low-dipping fracture zones beneath rock outcrops to a depth of 500 to 1000 m. The surface time-domain EM method has provided encouraging results for identifying the depth of highly saline pore waters.

The regional site scale investigations at the WRA included the drilling of twenty deep boreholes (> 500 m deep) at seven separate study areas. Geological core logging combined with borehole geophysical logging, TV/ATV logging, flowmeter logging and full waveform sonic logging in these boreholes helped to confirm the location of hydrogeologically important fractures, orient cores and infer the relative permeability of some fracture zones. Single-hole radar and crosshole seismic tomography surveys were useful to establish the continuity of fracture zones away from the boreholes up to distances of 50 to 400 metres. Single-hole hydraulic tests using straddle packer methods, testing in multiple-interval casing systems and large-scale crosshole pumping tests provided estimates of the in-situ permeability. Crosshole tracer tests were performed in several of the major fracture zones to estimate the solute transport properties and to provide information to scale up the properties to the regional modeling scale. Geochemical and hydrogeochemical characterization of host rock, fracture-infilling minerals, groundwaters and porewaters have provided data for flow modelling and safety assessment as well as obtaining supporting information such as groundwater ages, sources of salinity and rock-water interactions.

1 Introduction

AECL has been conducting detailed geological/geotechnical investigations in plutonic rocks at several Research Areas in the Canadian Shield since 1978 (Dormuth and Nuttall 1987). The main focus of the work was on developing and testing site evaluation and site characterization methods to investigate progressively larger volumes of plutonic rocks to depths of 1000 m. Major studies were conducted at Atikokan, Ontario (granite-granodiorite), Chalk River, Ontario (ortho- and paragneisses), East Bull Lake, Ontario (layered gabbroanorthosite), and Whiteshell, Manitoba (granite-granodiorite). AECL has also conducted brief field studies of about 30 other plutonic rock bodies on the Shield. One of the objectives has been to study the character and distribution of fracturing, at all scales, in several types of rock. A second objective has been to develop ways to analyze this information to infer conditions at depths of 500 - 1000 m to aid in the future siting of a nuclear fuel waste disposal vault. Both objectives help define rock conditions and characteristics for hydrogeological modeling. In this process, extremely detailed fracture and lithologic logging(including geophysical logging), and hydrogeological monitoring and testing of over 75 inclined boreholes (some drilled to depths up to 1 km) have been performed in the research areas. The 450 m-deep Underground Research Laboratory (URL) excavated in the Lac du Bonnet granite and boreholes in the associated Whiteshell Research Area have provided extensive opportunities to develop and demonstrate the area scale, site scale and local scale characterization methods. The results from the Lac du Bonnet Batholith (with twenty deep boreholes) are discussed in this paper. These results have been obtained by appropriate use of the disciplines of geology, geophysics, hydrogeology and hydrogeochemistry as described below. In the last two years this work has become integral part of Ontario Hydro's used fuel disposal program.

2 Geology

The Lac du Bonnet Batholith lies in the southern part of the English River Subprovince, the Winnipeg River batholith zone. The batholith is in sharp contact with the Bird River Greenstone Belt to the north and in gradational contact with foliated tonalite- granodiorite gneisses and migmatite. The batholith trends east-northeast, with about 1500 km² exposed east of the Paleozoic rock cover. The initial fault/fracture identification shown in figure 1 is partly based on several types of satellite data, airborne geophysical data, airphoto data and available bedrock geology maps. This is followed by detailed surface geological mapping, ground geophysics, surface hydrological and associated studies. The geology of the URL site is representative of the batholith as a whole. The gross structure, the variations in its largescale litho-structural components, and the orientation of smaller scale fabric elements affect the distribution of some of the fractures and large low-dipping fault zones. AECL mapped the batholith for category, lithology and fracture frequency at a scale of 1:50,000 (Brown and Thivierge 1981 and McCrank 1985) and the URL site for lithology and fracture characteristics and distribution at a scale of 1:1000 (Stone et al. 1984). Detailed geological work at URL site and five other smaller areas 'A', 'B', 'D', 'G' and 'J' shown in figure 1 has continued (Davison et al. 1994).

2.1 Lithology

The component granite phases of the batholith are pink, porphyritic granite- granodiorite, xenolith-bearing granite and grey granite. A pink, medium to coarse-grained, porphyritic granite underlies most of the lease site near surface at URL, site 'A', 'B' and 'D'. The site 'G' is at the southern contact of the batholith with tonalite the gneisses and site J is entirely in the gneissic belt. A grey granite that is commonly homogeneous and equigranular underlies much of the lease area below the sites exclusively in batholith. This grey granite is also found outcropping south of the shaft.

The alteration of the granite has been divided into five types: (*i*) three major, partially coinciding with petrologic units; and (*ii*) two minor, largely coincident with fracture zones (Brown et al. 1989). At the URL lease site and sites 'A', 'B' and 'D' the gross sequence from deep to shallow level is (1) grey granite, (2) green-grey granite, and (3) pink granite. Discrete zones of deep-red granite and clay rich granite occur in both units in association with fracturing in fault or other heterogeneous zones. Grey granite represents the mass of the batholith, with almost unaltered microcline, plagioclase, and biotite. The green-grey granite is similar, but epidote partially replaces plagioclase and biotite and the granite contains microscopic, chlorite filled fractures.

At the URL site shown in figure 2, pink granite is present from surface to a depth of 260 m. Grey granite underlies most of the pink granite away from fault zones. The intensity of pink coloration increases both towards individual fractures and also as the total number of fractures increases, suggesting that pink granite has further altered to dark red granite in the highly fractured zones and that the hydrothermal flow through these zones involved a large component of meteoric water. The compositional layering on a scale of 0.25 m to several tens of metres is common and is shown by variation in the contents of plagioclase, potassium feldspar, quartz and above all, biotite. The western half of the URL lease is underlain by a series of domes trending north-northeast in a long antiform and outlined by bands of xenolith-bearing granite and associated pegmatodial granite.

2.2 Structure

The formation of faults and mesoscopic fractures that are not filled by magmatic material appears to have been initiated immediately following the formation of the foliations, dykes, and quartz veins. At the URL site, fractures either are subvertical or dip 10-30°. Subvertical fractures, described in more detail are grouped into those striking north-northeast (015-020°), those striking east-southeast-southeast (110-130°) and those striking south-southeast (160-170°). The overall observations suggest a north-northeast trending maximum compressive stress and a vertical intermediate compressive stress axis at the time of fracturing, similar to the stress field during the formation of the later pegmatite dykes and quartz veins. Except in the vicinity of low-dip fault zones, subvertical joints striking east-southeast largely die out around 100 to 150 m from the surface, implying that they are only due to near-surface general extension, from whatever cause.

Low-intermediate-dipping (10-30°) fractures are common at surface and are associated with fault zones in the subsurface. There is a general tendency throughout the batholith for two pairs of thrust-movement fractures to form about north-north-east and southeast strikes. At the URL site three reverse faults, important in controlling groundwater flow, have been

encountered by drilling. Fracture zone 3 (FZ3) and a splay zone off fracture zone 2 (FZ2) were intersected in the URL shaft. FZ2 which was initially defined by drilling only was indicated in surface seismic reflection (Kim et al. 1994) and crosshole seismic tomography surveys (Wong et al. 1985). In characteristics these faults studied in detail at URL are typical of faults in the entire batholith.

3 Geophysical Investigations

Airborne magnetic data have been very effective in mapping the boundaries of granite rock masses and their contact with adjoining gneisses in the entire Superior Province. The Lac du Bonnet Batholith boundaries are clearly marked by the transition from a high total magnetic field, associated with granite/granodiorite mass, to a low magnetic field, mapped over gneisses to the north and south (Soonawala et al. 1990). In addition, the vertical magnetic gradient derived from the total field map has identified steeply dipping lineaments and lateral displacements along north north-east trending faults. The east south-east trending gradient anomalies are indicative of granodiorite dykes and near-surface concentration of xenolith-rich trends. Near-surface outcrops of FZ2 and FZ3 at URL study area are marked by magnetic lows on the total field map and identified in surface VLF-EM anomaly maps. Multi-frequency airborne EM data has been very useful in producing an overburden thickness map over the entire batholith (Dvorak 1988). In general most of the batholith is covered with thin overburden of 2 to 5 m thickness. One north-north-east 60 m thick sediment filled valley (the Dead Creek lineament) runs along a magnetic displacement anomaly. The Lee River is identified as another parallel magnetic lineament and supported by increased thickness of sediments in the airborne EM overburden map. The Lac du Bonnet and Rice Lakes have also been interpreted to have 15 to 60 m thick sediments. The surface gravity surveys have a mapped negative anomaly of up to 7 mgal associated with the batholith with a steeper gradient towards its southern contact with gneisses. The combined gravity and magnetic modeling along a few northwest- southeast cross sections (utilizing density and magnetic susceptibility values determined from a large number of surface samples from different rock units) indicate that the root of this batholith extends up to a depth of 15 to 18 kms (Tomsons et al. 1995).

Localized ground penetrating radar surveys over exposed outcrops have been very useful in mapping low dipping fracture zones to depths of 10 to 70 m. The regional seismic reflection profiles have identified scattered reflectors in depth range of 250 to 1200 m. However, in view of the increased ground noise in shallow surface seismic reflection data over crystalline rocks, the reflectors identified are at times ambiguous. Recent tests with time domain electromagnetic methods at the WRA (Maris et al. 1998) suggest that properly planned surface surveys can be used to identify the depth and lateral extent of regions of highly saline pore water saturated granitic rocks in the Canadian Shield environment.

The conventional geophysical logging tools and development of dedicated new logging tools like borehole radar and crosshole seismic tomography surveys have been extremely useful in detailed fracture mapping and lithologic logging (in association with the oriented cores) from many boreholes drilled to depths of up to 1 km. The conventional single-hole geophysical logging, supplemented by full waveform sonic, TV/ATV and core logging from all the 40 boreholes in this batholith (of which 20 are deep boreholes varying between 500 to 1000 m) has demonstrated that the upper 150 to 300 m of rock was a pink, fractured granite. Below

the upper pink layer, the rock is a sparsely fractured grey granite. The transition zone from the upper, moderately fractured rock matrix to deeper sparsely fractured rock may extend from few tens of meters to one hundred meters and more depending upon the locations of low dipping fractures and local lithological variations. Discrete, low- to intermediate-dipping fracture zones (10-75 m thick) have been encountered at depths of 200 to 1000 m. Epidote fillings have been found in a steeply-dipping fracture zone extending from the surface to at least 700 m depth in the grey granite at the B-site.

Conventional geophysical logging has been able to map fractures in a radius of 15 to 30 cm around the borehole walls. The reflections mapped by single-hole radar surveys were able to trace open fractures (identified in boreholes from core log or conventional logs) up to a radial distance of 60 m in the pink granite section of the borehole walls. The effective radius of investigation at greater depths (beyond 150 to 200 m) was found to decrease exponentially due to the reduced resistivity of grey granite caused by saturation of pore space by saline water.

Cross hole radar tomography surveys were able to map continuity of an intermediate-dipping fracture up to a distance of 100 m between boreholes WB1 and WB2 to a depth of 190 m. In the same pair of boreholes, the crosshole seismic tomography survey at a frequency of 4500 Hz shown in figure 5 was able to map two regions of low P-wave velocity (5400-5700 m/s) between depths of 150-220 m and 280-310 m (Lodha et al. 1991). The upper low-velocity zone mapped a fracture zone within pink granite. The lower, low-velocity zone represents another low-dipping fracture zone and the transition from pink to grey granite. Crosshole hydraulic testing demonstrated these fracture zones to be connected with the transmissivity values varying between 1.5×10^{-8} to 1.3×10^{-5} m²/sec. Below these two fracture zones the average P-wave velocity was 5850 m/sec which based on the core logs from these two boreholes and an understanding of velocity measurements at the nearby URL represents sparsely fractured, grey granite. A geologically-extrapolated epidote dyke exists between the two boreholes. However this feature did not produce any velocity anomaly in the seismic tomography panel and it showed no evidence of hydraulic conductivity in crosshole testing.

The crosshole seismic tomography tool developed in the CNFWMP/ UFDP to use in properly planned co-planner boreholes, has the potential of mapping the continuity of fracture zones and the volume of sparsely fractured rock to distances ranging from 200 to 400 meters up to 1000 metres depth. At the other extreme the small scale high frequency (10,000 to 20,000 Hz) crosshole seismic transducers, have been successfully used to measure excavation damage of 10 to 50 cm from the excavated walls at depths of 400 m in URL. The single hole radar, crosshole radar and crosshole seismic tomography techniques have been used in many small scale to intermediate scale experiments in the URL to characterize moderately and sparsely fractured rock, map fracture geometry behind excavated rooms, and to understand excavation damage zone in underground openings of different shapes (Hayles et al. 1995a, 1995b).

4 Geochemical Characterization

It is important to obtain an indication of the residence times ('ages') of groundwaters and get a semi-quantitative insight into rock-water interactions, rates of groundwater flow and the locations of modern and ancient flow paths. This, in turn, is used to provide qualitative support for the predictions of radionuclide-transport models.

In addition to siting requirements, for performance assessment modelling it is important to know the groundwater chemistry of the site because:

- 1. the total dissolved solids (TDS) content affects the density and viscosity of the groundwater;
- 2. the performance of the used fuel container and surrounding buffer materials is influenced by groundwater composition; and,
- 3. the retardation or migration of radionuclides with respect to buffer, backfill and various rock minerals is affected by varying pH, Eh and ionic strength conditions, and the presence or absence of specific dissolved components (e.g., HCO₃, F, SiO₂).

The parameters that were determined in characterizing the groundwater composition in Canadian program are shown in Table 1. In general, the pH, Eh and elemental concentration data were used in determining rock-water interactions that have occurred. The isotopic data were used to further delineate rock-water interactions and to determine the relative 'age' of the groundwater. Some typical rock-water interactions that were recognized as occurring in felsic igneous rocks were the carbonic acid attack and hydrolysis of plagioclase and orthoclase feldspars to produce kaolinite, illite and Ca²⁺, Na⁺, K⁺, SiO₂ and HCO₃⁻ in solution, carbonic acid dissolution of biotite to give kaolinite and $SO_4^{2^-}$. In addition, secondary minerals in fractures in the rock, such as gypsum and calcite may have been dissolved to give Ca²⁺, SO₄²⁻ and HCO₃⁻ in solution.

The composition of groundwater in most rocks of the Canadian Shield evolves from a dilute (TDS < 0.3 g/L) Ca-HCO₃ water in shallow bedrock in recharge areas to a highly saline (TDS ~ 50 g/L) Na-Ca-Cl or Ca-Na-Cl water at a depth of about 1 km. The variation in type and concentration of the major dissolved species in these groundwaters in the Canadian program in general and in particular at the URL lease area are shown in figures 3 and 4 respectively.

The process of chemical evolution of these groundwaters is complicated by mixing with deeper, more saline groundwater and rock pore fluids, whose composition may not be derived entirely from reaction with the granitic host rock. For instance, to the west of the Lac du Bonnet Batholith, in the Paleozoic sedimentary rocks of western Manitoba, are Na-Cl formation brines which may have penetrated eastwards into the granite under past hydrogeological regimes (Gascoyne et al. 1989). Isotopic analyses have helped to resolve the origin and residence times of these types of groundwater. Shallow, fresh groundwaters are essentially post-glacial in origin (less than about 8000 years old) whereas the intermediate-depth brackish waters contain pockets of cold-climate recharge which are probably of Late Pleistocene age. Underlying, saline groundwaters appear to be recharge that occurred under warm climate conditions and are probably pre-Pleistocene (>2 million years) in age (Gascoyne 1994).

Category	Species/Element	Category	Species/Element
Anions	HCO ₃ , SO ₄ , Cl, Br, F, NO ₃ , I	Sulphate Isotopes	S ¹⁸ O ₄ , ³⁴ SO ₄
Cations	Na, Ca, Mg, K, Sr, Si, B	Halogen Isotopes	³⁶ Cl, ¹²⁹ I
Trace Elements	Li, Fe, Mn, V, Al + Others	Strontium Isotopes	⁸⁷ Sr/ ⁸⁶ Sr
Dissolved Organic Carbon	Organic C	Uranium and Radium Isotopes	U, ²³⁴ U/ ²³⁸ U, ²²⁶ Ra
Colloids	Colloidal Fractions	Radon	²²² Rn
Environmental Isotopes	² H, ³ H, ¹⁸ O,	Dissolved Gases	H ₂ , He, O ₂ , N ₂ , CO ₂ , CH ₄ , Ar, H ₂ S
Carbon Isotopes	¹³ C, ¹⁴ C	Dissolved Inert Gas Isotopes	He, ³ He/ ⁴ He, ²² Ne/ ²¹ Ne

Table 1Summary of categories of samples taken and analyses made for
groundwaters collected in AECL's hydrogeochemical program.

5 Hydrogeological Characterization and Modelling

The rate, direction and chemical characteristics of groundwater flow through plutonic rocks of the Canadian Shield is controlled by the fracture networks that exist in the rock, their geometry and interconnections, and how the fractures connect to the surface topography. AECL has studied groundwater flow in plutonic rocks to depths of about 1 km at various geologic research areas on the Shield. These studies reveal that the degree of fracturing is the main distinguishing feature between domains of rock that have different groundwater flow characteristics. These domains comprise: zones of intensely fractured rock; regions of moderately fractured rock; and, low-permeability, sparsely fractured areas (figure 2) where the rock contains few, if any permeable fractures (Davison et al. 1990).

Field investigations show that the fracture zones are the most important pathways for the large-scale movement of groundwater and solutes through the rocks. These are narrow zones of intense fracturing that can be hydraulically continuous over relatively large distances and to great depths in the rock. These zones are often more permeable than the rest of the rock mass, although significant spatial variations in permeability can occur within them. In some cases the permeability range has been as much as six orders of magnitude $(10^{-12} \text{ to } 10^{-18} \text{ m}^2)$ over distances of a few metres and long interconnected channels of high permeability have been observed (Davison and Kozak 1989, Davison et al. 1990).

The regions of moderately fractured rock occur adjacent to the fracture zones as well as at shallow depths in the rocks. The frequency of permeable fractures associated with these domains of moderate fracturing decreases with depth and the rocks below a few hundred metres contain very few permeable fractures aside from the fracture zones.

Rock with very low permeability (less than 10^{-19} m^2) has been encountered below depths of 300 m to 800 m at all the geologic research areas examined so far. Studies at the Whiteshell Research Area reveal that domains of extremely low permeability, sparsely fractured rock greater than 500 m thick occur in the granitic Lac du Bonnet batholith below depths of only a few hundred metres (figure 6). Permeabilities as low as 10^{-22} m^2 have been determined from

hydraulic tests and abnormally high fresh water equivalent fluid pressures are recorded in piezometers that isolate these regions of rock. The high fluid pressures appear to be related to extremely high salinity pore fluids (up to 200 g/L TDS) that reside in the very low permeability rock (Stevenson et al. 1996a, 1996b).

Modelling studies were performed during construction of the revised groundwater flow model of the WRA to determine if the high fluid pressures in the domains of massive, sparsely fractured grey granite could be accounted for by the presence of dense, saline pore fluids. The modelling showed that if highly-saline $CaCl_2$ brine (up to 200 g/L TDS) occupied the pore spaces in these domains, most of the high fluid pressures could be explained. This explanation is supported by independent evidence from the URL site where samples of very slow seepage into boreholes drilled into domains of low permeability, sparsely fractured grey granite at the 420 m level show that the pore fluids are of $CaCl_2$ composition and have a salinity of at least 90 g/L (Gascoyne et al. 1996).

The results of modelling (Ophori et al. 1996) using the calibrated flow model were also analyzed and used to define boundaries for a smaller local model surrounding the selected, hydraulically-favourable location for a hypothetical disposal vault. In this analysis, several hydraulic cross sections were constructed across the flow model. Zones in which flow was either divergent or convergent were identified and assumed to be natural flow divides. Some of the divides were then connected to demarcate an area of about 75 km² for the revised local model around the selected, hydraulically-favourable location for a hypothetical vault. Groundwater flow in this local model region would need to be analyzed in much more detail as part of any process of developing a geosphere model for use in evaluating the overall performance of a hypothetical disposal vault at this location.

6 Summary

The entire geoscience/geotechnical process of site screening, evaluation and characterization of the disposal site is shown in figure 7. The integrated geological, geophysical, hydrological, hydrogeological and hydrogeochemical process begins with regional scale site screening-evaluation of a 500 to 1000 km² area selected from other considerations (volunteerism, socio-economic, geotechnical etc.). This process progresses with little overlap, between site screening and site evaluation activities, to site scale evaluation of smaller grid blocks (5 to 25 km^2) within the candidate area. This site scale evaluation involves more detailed investigations, such as drilling, in addition to surface-based investigations. The surface and subsurface information is integrated to produce a regional hydrogeological model with a depth of one to four kilometers. This regional model is then used to select a technically preferred location for the disposal vault.

The preferred vault location (about 5 km^2) is then characterized in detail to develop a threedimensional subsurface structural and groundwater flow model in preparation for vault design and performance assessment. All this information will ultimately be required to obtain a license for shaft sinking, underground excavation and vault characterization.

The detailed geoscience/geotechnical investigations completed at WRA and experiences from other studies provide enough support to suggest that reasonably large volumes of sparsely fractured plutonic rocks are present in the Canadian Shield. The knowledge gained in the WRA and URL clearly demonstrates that these sparsely fractured rocks, enveloped by low-

dipping and occasional vertical fracturing, can have very low permeabilities ($< 10^{-20} \text{ m}^2$). The hydrogeochemistry studies of groundwater from fracture zones and the rock matrix provide evidence of high salinity (> 50 g/L) fluids and, both late to pre-Pleistocene origin (> 2 million years in age) for these waters. This demonstrates that a long residence time of ground water in sparsely fractured volumes of plutonic rock can potentially provide a suitable environment for siting a safe repository.

The examples provided from WRA studies also demonstrate that geoscience/geotechnical application methods have enough resolution to identify saline water-saturated, sparsely fractured rock volumes and associated major fracture zones in plutonic rocks. The detailed site characterization methods are sufficiently advanced to develop subsurface structure and groundwater flow models for performance assessment and safety analysis for vault design. Any future developments in site characterization technology will provide additional enhancement for siting a nuclear fuel waste repository.

7 Acknowledgements

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FIGURE 1. Prominent Composite Lineaments from Remote Sensing Data (Airphoto, Aeromag and LANDSAT), Boundary of Regional Hydrological Study and Individual Smaller Site Evaluation Grid Blocks in the Whiteshell Research Area



FIGURE 2: The Three Main Fracture Domains in the WRA; a) Fracture Zones (faults), b) Moderately Fractured Rock, and c) Sparsely Fractured Rock



FIGURE 3: Generalized Evolution of Groundwater Chemistry with Flow Through Crystalline Rock Showing Typical Ranges of Salinity (TDS) Encountered at Depth



FIGURE 4: Schematic Cross-section Through the URL Area Showing Inclined Fracture Zones and Groundwater Chemistry in the Fracture Zones. Flow directions from pre- and post-excavation head distributions.



FIGURE 5: Cross-Hole Seismic Image of the P-Wave Velocity Between Boreholes WB1 and WB2 with Hydraulic Test Correlation. Histograms of the fractures observed in the core log are also shown. Low Velocity zones A1, A2, B1, B2, and C have increased hydraulic transmissivity (m²/s) compared to sparsely fractured rock transmissivity (D).



FIGURE 6: A Schematic Section of the Permeability, Porosity and Salinity Distributions in the Fracture Zones, Moderately and Sparsely Fractured Rock with Depth at WRA



FIGURE 7: Site Evaluation and Characterization Procedure for Constructing the Regional Conceptual Hydrogeologic Model and Selecting Preferred Vault Site. Detailed subsurface lithostructural and hydrogeological models are needed at selected site for ultimate vault design and performance assessment.

THE MIZUNAMI UNDERGROUND RESEARCH LABORATORY IN JAPAN -PROGRAMME FOR STUDY OF THE DEEP GEOLOGICAL ENVIRONMENT-

Hideki Sakuma*, Kozo Sugihara*, Kaoru Koide*, Shinichiro Mikake* and Göran Bäckblom**

- * Power Reactor and Nuclear Fuel Development Corporation, Tono Geoscience Center, Japan.
- ** Swedish Nuclear Fuel and Waste Management Corporation, Sweden. (Presently at PNC, Japan).

Abstract

This paper is an overview of the PNC's Mizunami Underground Research Laboratory project in Mizunami city, central Japan. The Mizunami Underground Research Laboratory now will succeed the Kamaishi Mine as the main facility for the geoscientific study of the crystalline environment. The site will never be considered as a site for a repository.

The surface-based investigations, planned to continue for some 5 years commenced in the autumn 1997. The construction of the facility to the depth of 1000 m is currently planned to:

- develop comprehensive investigation techniques for geological environment
- acquire data on the deep geological environment and to
- develop a range of engineering techniques for deep underground application

Besides PNC research, the facility will also be used to promote deeper understanding of earthquakes, to perform experiments under micro-gravity conditions etc.

The geology of the site is as shortly as follows: The sedimentary overburden some 20 - 100 m in thickness is of age 2 - 20 million years. The basement granite is approximately 70 million years. A reverse fault is crosscutting the site. The identified fault offers interesting possibilities for important research.

Part of the work during the surface-based investigations, is to drill and test deep boreholes to a planned depth up to 2000 m. Based on the investigations, predictions will be made what geological environment will be encountered during the Construction Phase. Also the effect of construction will be predicted. Methodology for evaluation of predictions will be established.

1 Introduction

One of the features of the programme for geological disposal in Japan is the establishment of research facilities. Such (Citations in italic, [...] is omission of the citation) facilities deep in the ground will serve as a common research base for geological disposal (Op.cit /AEC, Japan, 1994/). Detailed government guide-lines have been issued for the R&D in progress stating e.g. it is important to construct such research facilities at more than one location [...] focusing on both sedimentary and crystalline rock types as being representative of geology of Japan (op.cit /AEC, Japan, 1997/). The guide-lines also acknowledges the need for research on the engineered barriers in an appropriate scale. One major facility for such is the ENTRY facility in Japan c.f. /S.Masuda, et al. 1998/.

This paper is focused on the plans to construct an underground research laboratory in the crystalline rock in Japan. As part of the preparations for such a laboratory PNC has been participating in Underground Research Laboratory projects in Belgium, Canada, Sweden and Switzerland. Substantial work has been conducted concurrently in Japan, particularly at the Tono and the Kamaishi mines, to obtain basic understanding on the geological environment and to test and develop the basic technology to be applied for the Japanese geological environment.

The overall ambition of The Mizunami Underground Research Laboratory is to develop the facility into an international center of excellence. The site about 350 km west of Tokyo, Fig 1, will never be considered as a potential site to host a geological repository. The surface-based investigations, planned to continue for some 5 years commenced in the autumn 1997. The construction of the facility to the depth of 1000 m is currently planned for the purpose mentioned earlier. Besides PNC research, the facility will also be used to promote deeper understanding of earthquakes, to perform experiments under micro-gravity conditions etc.

2 Developments in the Japanese Policy for Nuclear Energy and Geological Disposal

The Japanese policy on nuclear energy is outlined in documents issued by the Japan Atomic Energy Commission (JAEC). From the very beginning the overall element in Japan's nuclear energy policy has been to establish a nuclear fuel cycle extending from securing of uranium resources to disposal of radioactive waste. As to the disposal of high-level waste, the generic R&D work conducted by PNC and other agencies is as already decided 1992, clearly separated from any work for the implementation of the geological disposal.

The Japan Atomic Energy Commission updated 1994 the long-term programme on nuclear energy /AEC, Japan, 1994/. The general aims of the revised programme are a long-term programme that:

- will be met by understanding of the Japanese public,
- will be met by understanding internationally,
- provides concrete guide-lines for those involved in development and utilization of nuclear energy.

With respect to the back-end measures it is clearly stated that the national government is responsible for adopting appropriate measures to ultimately ensure that those responsible meet their responsibilities regarding safety. That includes comprehensive formulation of disposal methods, confirmation of the safety of the disposal and devising of legal and other measures that are necessary for long-term guarantee of meeting of responsibilities regarding disposal.

The tentative target for commissioning of the repository is slated for year 2030 - 2045, but pending conditions. As to provide the scientific and technological basis for geological disposal research facilities deep underground will serve for:

- accurate determination of characteristics and features that should be taken into consideration
- enhancement of the reliability of the models for evaluation of the performance of the system contribution to Japan's scientific research on the geology of deep strata

The PNC is assigned to publish and submit to the government the second progress report on the research and development of geological disposal before the year 2000. The first /PNC, 1992/ was submitted. The Guide-lines published /AEC, Japan, 1997/ provide details on the scope of the report. PNC is assigned to demonstrate more rigorously and transparently the feasibility of the disposal concept. The 2nd Progress Report will be internationally reviewed before submitting to the Japanese Government.

3 Involvement in Research on the Geological Environment

PNC has since long recognized the benefit of international cooperation in the field of research and development on geological disposal. Participation in URLs has been an integral part of the PNC R&D Programme. The experience gained from the participation of URLs has been of very high importance for execution of the work in Japan. Table 1 provides an overview of past, current and planned activities relevant to URLs. PNC participated in the OECD/NEA Stripa Project 1980- 1992 /C.Fairhurst, 1993/. Important contributions were the development of instruments and procedures to characterize the geological environment and the increased understanding of groundwater flow and transport of solutes demonstrated by evaluation of predictive modelling of experiments. The Stripa Project provided a valuable technological basis for the similar studies performed in the Kamaishi Mine. At the Kamaishi Mine research on the geological environment has been focused on detailed characterization of the geological conditions, the excavation disturbed zone, studies on transport of solutes and influence

of earthquakes on the geological environment /T.Sato, 1996/. Experience in the Swiss Grimsel Test Site, Swedish Äspö Hard Rock Laboratory and the Canadian Underground Research Laboratory has e.g. been referred to in the detailed planning of research such as transport of solutes and the excavation disturbed zone. All field research activities in the Kamaishi Mine was however closed down in March 1998 as the agreement set up between PNC and the Kamaishi Municipality expire. The Mizunami Underground Research Laboratory now will succeed the Kamaishi Mine as the main facility for the geoscientific study of the crystalline environment.

With respect to the geoscientific study of the sedimentary rock, PNC has been involved in the Belgian Underground Research Facility (URF). The ongoing participation in the international Mt. Terri project /1997/ together with the extensive work in the Tono Mine /T.Sato, 1996/ will be most valuable for planning of an underground research laboratory in the sedimentary environment in Japan. The current plan is to construct such a laboratory in Horonobe, Hokkaido. The sites for the MIU- and the Horonobelaboratories will not come into consideration as repository sites.

The MIU project will, to some extent, duplicate similar work conducted previously in Canada and Sweden. The Table 2 provides some overview of similarities and differences in this respect. It is evident that PNC can utilize 10-15 years of previous experiences from Canada, Sweden and elsewhere in the planning.

4 Outline of the Mizunami Underground Research Laboratory Project

4.1 Permits

The need for an underground research facility to study the geological environment is firmly established. As explained before, there is a very clear separation between the general R&D on geological disposal and the work needed for implementation of the geological disposal. The general public, in particular those who live near the laboratory site, anyhow have concern that an underground research laboratory somehow later can be converted to a geological repository.

4.2 Site

An overall evaluation for siting the URL led to the decision to site the URL in Mizunami City. The area of the land is 140,000 m². According to the current plan, all facilities will be constructed within the boundaries of the PNC land.

4.3 Objectives

The main goals of the MIU are to:

1. Develop comprehensive investigation techniques for geological environment, i.e. to systematically combine fundamental methodologies developed to demonstrate the effectiveness of technology for reliable investigations, predictions and models of the characteristics of the geological environment.

2. Acquire data on the deep geological environment,

High-quality data will be collected to improve the reliability of models of geology and groundwater flow, to evaluate engineering materials for underground construction and operation.

3. Develop a range of engineering techniques for deep underground application, i.e. to evaluate techniques for design and construction of large-scale facilities underground and to clarify the potential long-term effects of these techniques on the geological environment. Studies for managing safety and operating environment in such underground facilities are also planned for.

Stage goals for the Surface-Based Investigation Phase, the Construction Phase and the Operating Phase have been set.

4.4 Scope of works

Part of the work during the surface-based investigations, is to drill and test 11 deep boreholes to a planned depth up to 2000 m. Based on the investigations, predictions will be made what geological environment will be encountered during the Construction Phase. Also the effect of construction will be predicted. Methodology for evaluation of predictions will be established.

4.5 Design

The design of the surface facilities is now in progress. It is planned that the shaft will be constructed to a depth of 1000 m with a diameter of 6 m. In addition to the shaft, the extension of the galleries are also considered. The detail design for the galleries will be decided according to the geological model from surface-based investigation and the research programme.

4.6 Schedule

Borehole drillings on the site commenced in November 5 1997. It is expected that the surface investigations will continue for 5 years. The construction is expected to last for 8 years. Experiments are planned for a period of 12 years. The total project duration thus planned for is some 20 years taking phase overlaps into consideration.

4.7 Miscellaneous

There is an overall ambition that the MIU will be developed into an international center of excellence. The MIU-facility will in accordance with the Gifu-Mizunami-Toki-PNC agreement be open for other types of research such as earthquake research and experiments under micro-gravity conditions.

5 Surface-based investigations

Some technical details from the planned investigations are presented. Given the size of the Shomasama site, the general strategy for boreholes is to investigate "outwards" from a possible shaft location. Due to the early construction of the surface facilities, the tentative shaft location will be decided upon very early in the investigations. Investigations will start by drilling some holes in the vicinity of the possible shaft location succeeded by boreholes at distances of several tens of meters to hundred meter.

5.1 Geological investigation

Magnetotelluric measurements will be done by about 150 point measurements. The frequency is in ranges between 1 and 100 kHz. Target depth is down to 1 km. Reflection seismic surveys will be planned for the following years.

Drilling is done to collect core samples as well as to perform a series of tests and measurements. No drilling mud is planned to be used. Tagging of drilling water will be made by uranine. The drilling water is re-circulated. Borehole deviation should be less than 1 degree per 100 m and 10 degrees in bottom of hole.

Cores are photographed. In connection with drilling, concurrent (manual) mapping is done. The following is recorded: Staff, altitude, depth, column and lithofacies, color tone, rock type, hardness, rock core shape, bedrock class, RQD, weathering, degeneration, fracture (shape, continuity, degeneration, fracture infilling material etc.), and miscellaneous.

Borehole geophysics is done by different logging tools. Resistivity is measured by Self-Potential measurements in the 20~300 Hz range. The formation density is measured by gamma-gamma logging. Other logs are neutron and natural gamma, sonic, temperature, caliper, radar (60 MHz antenna frequency) and diameter.

Fractures down to 0.1 mm in aperture will be recorded using a borehole TV. Interpretation is made of e.g. fracture location, strike, dip, aperture, frequency, fracture minerals etc. The results are displayed in stereographic projections and shown. Sample statistics is done.

5.2 Hydrogeological investigation

The following hydraulic tests are tentatively planned to be conducted in the boreholes;

- Drilling is discontinued every 100 m down to bottom. Pumping is done by conventional pumps or by airlift pumping. Pressure is recorded during fall off and recovery. Hydraulic transmissivity is evaluated by the Theis or Jacob-Lohman method.
- Flow-meter logging will be conducted for three different flow rate. The flow rate is kept for about 3 hours to inject. The pressure increase and fall off is measured so that the transmissivity of the complete hole is evaluated. The variations in the

spinner are used to pinpoint the position of conductive features and to evaluate the transmissivity distribution along the hole.

Packer tests are conducted in selected (conductive) sections of the borehole. Depending on hydraulic conductivity, either pulse tests or slug tests will be conducted. The pulse test is used for low conductive rock in the range 10⁻⁸ - 10⁻¹² m/s and the slug test in the range 10⁻⁶ - 10⁻⁹ m/s. The pulse tests are conducted by suddenly increasing the pressure. The fall-off after the pressure pulse is then measured up to some hour. The slug test is performed by injecting a rod into the packed-off section. After the "slug" the fall-off in pressure is recorded. Evaluation of conductivity is made by the Hvorslev method when the log pressure versus time is a straight line or the Cooper method when not.

5.3 Geochemical investigation

Water in the borehole is sampled by a special PNC probe/sampler. The maximum sampling volume is 500 ml, maximum pumping capacity 10 -100 ml/min. The probe measures pH (0-14), pS (Sulphide) (-1000 \sim 0 mV), Eh (-1000 \sim 1000 mV), temperature (0~50° C and electrical conductivity (0 ~ 100 000 S/cm).

5.4 Geomechanical investigation

Several types of tests are conducted to establish the physical properties, like effective porosity, water content and water content ratio, density (wet, natural, dry), specific gravity, unit product weight, seismic velocity, compressive strength, thermal conductivity specific heat capacity and coefficient of thermal expansion, magnetic susceptibility and specific resistance. Samples are also tested to determine mineralogy and to determine the primary rock stresses by methods of Acoustic Emission and Differential Rate Analysis.

5.5 Modelling work

The methods to be used for predictions, models and evaluation are still in the finalizing process, considering experiences achieved by relevant projects worldwide.

6 Concluding Remarks

Underground Research Laboratories play important roles in the national programmes for geological disposal in many countries reflecting the concept and progress of geological disposal. The MIU is an essential facility in Japan to broaden the knowledge-base, particularly in geoscience. The work at the PNC's Mizunami Underground Research Laboratory (MIU) will be planned and executed in accordance with the general goals of the Atomic Energy Commission so the MIU project will

- be met by understanding of the general public,
- be met by international support,

provide concrete scientific and technological results of importance for a safe geological disposal in Japan.

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YEAR	1980 - 1990	1990 - 2000	2000 -(tentative)
Government policy	Generic Research and Development	Generic Research and Development	Generic Research and Development Implementation
Sedimentary rock	Research in the Tono Mine Planning for a URL in Hokkaido	Research in the Tono Mine Planning for a URL in Hokkaido	Research in the Tono Mine Construction of a generic URL
	Participation in the Belgium HADES project 1987-1992	Participation in the Swiss Mt. Terri Project 1996 and onwards	Construction of a URL (by implementing organisation) at the site that may later be the repository site
Crystalline rock	Participation in the OECD-NEA Stripa Project from 1980 - 1992	Participation in the Swedish Äspö Hard Rock Laboratory from 1991 and onwards	
		Participation in the Canadian URL	

Table 1 OVERVIEW OF URL ACTIVITIES IN JAPAN (PNC)

I	Project from 1996 and onwards	
	Participation in the Swiss Grimsel Test Site from 1989 and onwards	
	The Kamaishi work will be closed down 1998	
Execution of research in the Kamaishi Mine from 1988 and onwards	Preparations for the Mizunami Underground Research Laboratory from 1995 and onwards	Construction and operation of the Mizunami Underground Research Laboratory

Table IICOMPARISON BETWEEN URL IN CANADA, JAPAN AND
SWEDEN

Decemintion/	Underground	Mizunomi LIDT	Asnö Hard Rock
Description/	Dagaarah	TADAN	Aspo naru Kock
Laboratory	Kesearch	JALAN	Laboratory
	Laboratory		SWEDEN
	CANADA		
Owner/Onerator	Atomic Energy of Canada	Power Reactor and Nuclear	Swedish Nuclear Fuel and Waste
	Limited (AECL)	Fuel Development Co(PNC)	Management Co (SKB)
Overall Purpose	Research facility to assess	Generic research to develop	Dress-rehearsal facility to test,
	feasibility and safety of deep	knowledge in deep geological	develop and demonstrate technology
	geological disposal of	environment and engineering	and models under realistic conditions
	nuclear fuel waste in	techniques	before application at a real repository
	plutonic rock.		site.
Host rock	Precambrian granitic	Granitic rock (70 Ma)	Precambrian granitic rock (1400 -
	batholith (2670 Ma)	covered by sedimentary rock	1800 Ma)
		(2-20 Ma)	
Main goals	The current (1998) are to:	The current (1998) are to:	The current (1998) are to:
1.1410 20412	1 Contribute to	I Establish comprehensive	1. Increase the scientific
	understanding of the	investigation technology for	understanding of the safety and
	fundamental mechanisms	geological environment	function of a repository
	affecting the rock mass and		
	groundwater system	2. Acquire data of deep	2. Develop and test technology that
		geological environment	will simplify disposal and decrease
	2 Demonstrate some of		costs while retaining quality and
	the technology necessary	3 Develop a base of	safety
	are reennoinely necessary	engineering techniques in	June 1
	3. Validate assumptions	deep underground	3. Demonstrate the technology that
	used in the disposal concept		will be used for disposal of spent fuel
			and other long-lived wastes
Major Score of	1. Solute transport studies	1. Development of	1. Development of integrated
iviajor Scope of		programme and plans for the	database and visualization system
Works (1997)	2 Vault sealing system	Surface-Based Investigation	
	studies	Phase and the provisional	2 Test of models for groundwater
		plan for the Construction	flow and radionuclide migration
	3 Radionuclide migration	Phase	
	etudies	1.1.00	3 Demonstration of technology for
		7 Borehole drilling and	and function of important parts of the
	A Excavation response	testing	repository system
	studies	i souris	
	Sunce		
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Schedule	Site investigations 1980- 1984 Construction Phase 1984- 1990	Surface-based investigations 1997-2001 Construction Phase 2002- 2008	Site investigations 1986-1990 Construction Phase 1990-1995 Operation Phase 1995-
Design	Shaft to 420 m depth. Shaft station at 130 level and 300 level. Galleries at 240 level and 420 level. One ventilation raise and several experimental drifts excavated	Shaft to ~ 1000m Depth to galleries and layout not decided yet	Access ramp 3600 m to depth 450 m, hoist raise and two ventilation raises. Several experimental drifts excavated
Construction	Excavation by drill and blast Some experimental excavations by mechanical methods	Excavation by drill and blast	Excavation of ramp by drill and blast 3080 m and mechanical excavation for 420 m. Raises excavated by raise drilling.
Current international cooperation (1998)	France, Japan, Sweden, USA	Plans are in progress	Canada, Finland, France, Germany, Japan, Spain, Switzerland, UK



Fig. 1 Location and a Conceptual View of the Laboratory

STRUCTURE AND USE OF CONCEPTUAL MODELS IN THE ÄSPÖ SITE INVESTIGATIONS

Gunnar Gustafson

Chalmers University of Technology, Sweden

Abstract

Early in the Äspö project a need for structuring and clarification of the models used for different purposes was identified. The problem lied not in the numerical codes or the data base used for the modelling but rather in the process of how the real world was conceptualised into descriptive and predictive models. A proposal on how to structure these conceptual assumptions was made on which a standardised representation of used models was worked out. An essential objective has been to condensate the model descriptions to one page and still present the essential aspects of each model. It is hoped that in this way it is easier to obtain an overview of the assumptions underlying each model and facilitate comparison between different models.

The base for the description is the *intended use of the model*. Based on the intended use the next step is to identify what *physical* processes should be included in the model. In some cases these processes can be represented by constitutive equations. The next step is to define the *concepts* needed to solve the problem. The concepts may be separated into four groups. Firstly, the type of *geometrical framework* and the framework-related parameters have to be defined. Secondly, the type of *material properties* to be assigned to the domains defined by the geometrical framework must be decided. Thirdly, the *spatial assignment method* of the material properties within a domain has to be described. Finally, the model normally has a limited extent and the *boundary conditions* have to be defined to compute or judge the effects within the model. For a real case the data can now be defined for the four groups of concepts by analysing measurements representing the actual case. If needed *a numerical or mathematical* tool that handles the processes and concepts should the be chosen. *Output parameters* of interest for model purposes must then be defined.

1 Introduction

The performance and the safety assessments of a repository for spent nuclear fuel needs to be based on a chain of models which describe the action of the natural and engineered barriers that confine the deposited high level waste. Each of these models summarises in some way the qualitative and quantitative knowledge, which we have for the repository area in such a way that we can consider it to be possible to judge its future behaviour.

The development of these models generally follows a number of steps during the course of a project. An important part of this evolution is the development of the conceptual models, defined as a set of assumptions used to describe a system for a given purpose. These assumptions concern the geometry and dimensionality of the system, and the nature of the physical and chemical processes.

2 Models in a scientific context

The basic theories of physics are based on a set of fundamental principles which are held to be generally valid by the scientific community. We may regard these principles as basic laws of nature. Examples of such laws are:

- conservation of energy
- conservation of mass
- conservation of charge
- principles of thermodynamics

Essentially, all theories describing specific phenomena and processes are based on, or have to be consistent with, these laws, see Figure 1. In this context we may define a theory as a description of the principles and relationships which control a specific process or group of processes.

To qualify as a theory, the principles and relationships should be assumed to have a general validity rather than be applicable only in specific situations. In this way a theory should provide a means for describing phenomena that occur under many different circumstances.

Thus in our view, there is an essential distinction between a theory and a model. A theory is expected to be generally applicable whereas a model is used to provide a representation of a process or a system for a specific purpose. Hence a model generally attempts to describe those aspects of nature which we think are important for the problem we wish to solve or the predictions we attempt to make. It should also be recognised that it is essentially in the definition of a model that approximations are introduced. Whether these approximations are valid or not has to be judged in relation to the purposes of the application.

3 Key issues and scales

Early on in the Äspö project there was a need to structure the work both with respect to the issue that was studied and on what scale the characterisation was done. This way five key issues were identified, each reflecting an important issue regarding repository safety. The geometrical scales were originally introduced because we very soon found out that the same level of detail could not be kept throughout the large rock volume that was of interest for the Äspö Laboratory.

3.1 Rationale behind key issues

The geological-structural model describes structures on different scales and represents a simplification of the real physical medium. The geological model forms the geometrical basis of all models of the geosphere, regardless of the processes described. The geological model not only forms the geometrical basis of the models, but is also of vital importance as decisions on the design of the repository will be influenced by it. A repository volume will in the future be selected to avoid major fracture zones. Deposition tunnels and spent fuel canisters will be positioned to avoid the major flow paths.

Mechanical stability of the rock mass is of interest both in a short and a long-term perspective. Mechanical stability is a necessary condition during construction. The long-term issue is to identify potential zones of movement, so that these can be avoided for emplacement of the spent fuel canisters.

Groundwater flow is an important factor that may influence the service life of the spent fuel canisters and the dissolution of the spent fuel. The description of the groundwater flow provides a necessary, but not sufficient, basis for calculating the transport of nuclides from the repository to the biosphere if the waste package should fail.

Hydrochemistry is an issue as the chemical situation influences the corrosion of the spent fuel canisters and the dissolution of the waste. Hydro chemistry provides a necessary, but not sufficient, basis for calculating the transport of nuclides from the repository if the spent fuel canisters should fail.

Transport of solutes provides a necessary, but not sufficient, basis for calculating radiation doses from a sealed final repository.

3.2 Rationale behind the geometrical scales

Characterisation on a *regional scale* >1000 m provides a basis for selecting a suitable rock volume for the repository and defining boundary conditions for the site scale. Areas of groundwater recharge and discharge can be defined. The regional assessment will provide a basis for long-term predictions of the future location of discharge areas as well as where potential zones of movement can be found.

The *site scale* characterisation, 100 - 1000 m, will be used to locate major fracture zones and/or major flow paths. These investigations are essential as they will provide guidance in determining the repository depth as well as the main layout of
the repository Characterisation on this scale also provides data to assess the farfield groundwater flow through the repository and flow paths to the biosphere

Block scale characterisation and data, 10 - 100 m, will be used for detailed layout of the repository. Safety assessments include the transport of solutes from a leaking waste package to major flow paths.

The *detailed scale*, 0 - 10 m, may be the most important scale, as properties on this scale define the geohydrological, chemical and mechanical near-field of the waste package. By proper selection of waste package positions it will be possible to provide the suitable environment for long-term isolation of the waste.

This definition of geometrical scales is, however, more or less subjective. It may also be pointed out that a real site is likely to be larger than a square kilometre and is of course not limited by the so-called site scale.

4 Model components

As described in the introduction, the performance and safety assessment for a repository consists of a series of modelling activities which together represent the function of the repository system as a whole Each sub-model in this sequence describes a process or a set of processes which are important for the overall performance of the system. For each of these models we must decide which physical processes are to be included. In this context, chemical processes are considered to be a sub-set of physical processes. These processes should be described by some generally accepted theory. If the theory is quantitative, it should include a mathematical formulation in terms of some directly, or indirectly, measurable quantities. The relation between these quantities can normally be described by a set of constitutive equations. The processes take place in an environment defined by a structural framework constrained by some boundary and initial conditions. All these factors can be e defined with differing degrees of generality. A model can thus be separated in a hierarchical way based upon the generality of the assumptions. We therefore propose the following distinction, which is based upon the definition given in the introduction:

- a *conceptual model* which defines the physical processes and the structural framework within which the problem is to be solved; this includes constitutive equations and boundary conditions.
- a *model realisation*, whereby data are introduced into the conceptual model and a numerical or analytical tool is used to compute the effects, i e to generate output.

One must, however, bear in mind that the development of the mathematical tool generally has to be closely coupled to the structural framework of the conceptual model. The choice of the computational approach will thus be far from arbitrary with respect to the realization.

In this context, the conceptual model becomes a relatively general description of the *way the model is constructed*. This should be regarded separately from any specific realisation of it. Hence a conceptual model should consist of:

- a scope for the modelling
- a specification of the *processes* (including constitutive equations) that are included in the description.
- a specification as to which way the model should be divided into *structural* units or entities.
- a specification as to how *boundary and initial conditions* are to be included in the model.
- a specification of the *parameters* (state, material and geometry) pertinent to the model.
- a specification of the principles as to how *assignment of parameters* is to be made for each of the structural units.

If needed a *mumerical or mathematical tool* that handles the processes and concepts should then be chosen. *Output parameters* of interest for model purposes must then be defined.

Behind these concepts lies rationale based on experience, logical reasoning and test procedures, but note also that the conceptual model may need to be different depending upon what behaviour we actually want to model in a particular problem.

5 The structure of conceptual models

In order to clarify the assumptions behind models used, a proposal of how to structure these assumptions was made in^1 . The structure is presented in *Table 1*. An essential objective has been to condense the model description to one page and still present the essential aspects of each model. It is hoped that in this way it will be easier to obtain an overview of the assumptions underlying each model and facilitate comparison between different models.

Table 1. Format for a condensed description of models in the Äspö HRL project'.

MODEL	NAME
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Model scope or purpose Specification of the intended use of the model

Process description Specification of the process accounted for in the model, definition of constitutive equations

CONCEPTS	DATA			
Geometrical framework and parameters				
Dimensionality and/or symmetry of model. Specification of what the geometrical (struc- tural) units of the model are and the associated geometrical parameters (the ones fixed implicitly in the model and the variable parameters).	Specification of the size of the modelled volume. Specification of the source of data for geometrical parameters (or geometrical structure). Specification of the size of the geometrical units and resolution.			
Material	properties			
Specification of the material parameters contained in the model (it should be possible to derive them from the process and geometrical units).	Specification of the source of data for material parameters (could often be the output from some other model). Specifica- tion of the value of material parameters			
Spatial assign	ment method			
Specification of the principles for the way in which material (and if applicable geometri- cal) parameters are assigned throughout the modelled volume.	Specification of the source of data for model, material and geometrical parameters as well as stochastic parameters. Spec- ification of the result of the spatial assign- ment.			
Boundary	conditions			
Specifications of (type of) boundary condi- tions for the modelled volume.	Specification of the source of data on boundary and initial conditions. Specification of the boundary and initial conditions.			
Numerical or ma Computer	athematical tool			

Output parameters Specification of the computed parameters and possibly derived parameters of interest.

6 The development of the conceptual model

Both in general terms and within a specific project, models and their concepts develop and thus change with time. The way this is done may be called updating, using an analogy with the terminology of Bayesian statistics.

This approach towards making progress is, in our belief, deeply rooted in the scientific and engineering methodology. So deeply is it rooted that it is applied in most cases and in more or less an intuitive way. So is the pre-investigation for the Äspö Hard Rock Laboratory² (ÄHRL). If we look at the regional and site scale groundwater modelling, we see that it has been developed in a stepwise manner from generic studies, leading on to development of a site scale model wherein the changes caused by the excavation of an access ramp could be predicted. In hindsight, one finds a reasonable logic to the development of the conceptual models, even if our analysis of the problems initially was far from strict. Overviews of the results at each of a number of different stages, and also of the conceptual models used, have been published in a series of evaluation reports^{3,4,5,6,7} for the ÄHRL, here named from their report numbers in the SKB series: TR 88-16 (Site-localisation stage), TR 89-16 (Site-investigation stage) and TR 91-22&23 (Site-characterisation and prediction stage). In *Table 2* we have tried to extract the overall concepts from the reports. We will now try to use that table to examine the progress of our modelling.

A quick look at the table shows that the list of concepts grows during the project. First of all we have to consider the lack of information that prevails at the early stage of a project. This means that even if we know that eventually we will have to model different features in detail, we have insufficient information to meaningfully do that at the beginning and therefore it is best to refrain in order to have a balance between input and output. The growth of the database for the area then both stimulates a development of the conceptual models and makes it feasible.

From the table, we find that we do not introduce every conceivable concept into the model, but only those for which we have a rational use to meet with a certain scope. In the best case, the rationale will be logic reasoning, statistical tests or professional experience, but also prejudice and preoccupation cause us to adopt concepts. Analysing of the rationale will thus stimulate development of the conceptual models. New scientific results or new phenomena, perhaps found in the course of the project or obtained from elsewhere, has played a lesser role than expected. In the case of ÄHRL, the reason for the introduction of conductive fracture zones in TR 89-16 is not that we were unaware of them before, but that we then knew too little about their properties to be able to incorporate them. However, if we look at a subset of the concepts of different types of fracture zones, new and important types have been identified which will exert a considerable influence on the transport modelling.

A more detailed and comprehensive scope for the model implies the need for further development of the concepts. This follows directly from the subtitles, so that the target is successively homed-in upon by characterisation and predictions made at the actual site.

Model stage	SKB TR 88-16 Regional flow modelling Gustafson et al /1988/	SKB TR 89-16 Regional flow modelling Gustafson et al /1989/	SKB TR 91-22 & 23 site scale modelling Wikberg et al, Gustafson et al /1991/
Scope	Natural flow Flow to underground laboratory	Natural flow Flow to underground laboratory Cross-hole tests (calibration)	Natural flow Flow to underground laboratory Cross-hole tests (calibration)
Processes	Darcian 2D flow	Darcian 3D flow Salinity	Darcian 3D flow Salinity
Structurai units	Homogeneous sub-volumes (lithology, depth)	Planar conductive fracture zones Homogeneous sub-volumes (lithology, depth)	Planar conductive fracture zones Stochastic continuum in sub-units (lithology, depth)
Boundaries	Constant head on top No flow for the rest	Constant head on top No flow for the rest	Top: Fixed recharge (land), constant head (water) Sides: Prescribed pressures Bottom: No flow Tunnel: Given pressures (with or without skin)
Parameters	Hydraulic conductivity Head on boundaries Space coordinates	Hydraulic conductivity Zone transmissivities Head on boundaries Space coordinates	Stochastic distributions for hydraulic conductivity Transmissivity (deterministic for each zone) Salinity linearly increasing with depth Heads and recharge rates on boundaries Space coordinates
Parameter assignment method	Inference from other areas Analysis or regional data Inference from generic modelling Boundary heads = topography	Inference from TR 88-16 modelling Analysis or regional data Site specific conductivity data Boundary heads = topography	Inference from TR 89-16 modelling Analysis of regional data Site specific conductivity data Site specific transmissivity data Water chemistry data Recharge from sensitivity studies Calibrations

Table 2. Conceptual models in regional and site scale modelling for the Aspö Hard Rock Laboratory

7 Accepting or discarding concepts

Every model step is made from an update of the previous model. Old concepts have to be revised as new information is acquired and as new concepts are added. Special attention nevertheless has to be given to those major changes where we have been shown to be wrong. When printed as a table such as *Table 2*, it is not possible to see such mistakes, but for example our ideas concerning the depth dependence of hydraulic conductivity start up as a simple logarithmic decline, but this had to be changed radically as the first generic models evoluted towards the final site-model in which we rely more heavily on rock-type and tectonic setting. It is not always easy to discard concepts, which you have once believed in and became familiar with.

The question of which criteria to use, as to what to accept, keep or discard when dealing with a conceptual model is not easily answered. We definitely believe that it is impossible to set up quantitative or formal criteria. Our practical suggestion is to take a more pragmatic approach whereby we try to identify those good things which will follow if we adopt the concept in question. We propose that each conceptual model should be analysed with respect to its usefulness and feasibility. We suggest the establishment of a set of questions such as the following which can be used to sift or sort out those concepts which should be kept from those which should be rejected:

Are the concepts useful:

- Do they reflect the physics behind your problem sufficiently well?
- Do they describe the model area in a way that reflects your knowledge about it?
- Do they make it possible to model the requested parameters with an acceptable accuracy?

Are the concepts feasible:

- Has the simplest set of concepts been used to describe your problem in relation to the data available?
- Can parameter values be assessed with reasonable effort?
- Do they give robust results?

The list can be made more comprehensive and needs to be discussed and revised, but we believe that this may be a good approach towards finding out whether or not you have an appropriate set of concepts in your model.

Finally, the very first model is worth some reflection. What was the origin of the very first model? One can specify experience, generic modelling and professional judgement, but also prejudice and preoccupation. We believe that this is a fact with which we have to live. It is not easy to define the "start" since many of the processes described here are self referential, semi-intuitive and may even be creative. The important point, however, is that we are able, with an open but critical mind, to let the conceptual models grow and develop. With a travesty of an old saying: It is the way, not the start, that is of importance to achieve the goal.

10 References

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⁶ Gustafson G, Liedholm M, Rhén I, Stanfors R, Wikberg P, 1991: "Äspö Hard Rock Laboratory, Predictions Prior to Excavation and the Process of their Validation". SKB TR 91-23, Stockholm

⁷ Rhén I ed, Gustafson G, Stanfors R, Wikberg P:"ÄSPÖ HRL – Geoscientific evaluation 1977/5 Models based on site characterization 1986 – 1995". SKB TR 97-06, Stockholm.

MODEL 96 OF THE ÄSPÖ SITE. RESULTS OF PREDICTION AND OUTCOME BASED ON SURFACE AND UNDERGROUND BORE HOLE INVESTIGATIONS

Ingvar Rhén , Gunnar Gustafsson, Roy Stanfors Peter Wikberg VBB VIAK, Göteborg, Sweden CTH / VBB VIAK, Göteborg, Sweden RS Consulting, Lund, Sweden SKB, Stockholm, Sweden

Abstract

The site characterisation work of the bedrock around Äspö has been carried out as an interdisciplinary work in the fields of geology hydrogeology and hydrochemistry. It has been carried out in different steps focusing on different scales simultaneously. The descriptions have been focused on regional, site and block scales representing areas/volumes of 10x20 km, 500x500x500 m and 50x50x50 m respectively during the pre-construction phase. During the tunnel construction phase the models have been focusing scales of 0-10, 10-100 and 100-1000 metres.

The models after the pre-investigation stage were the base for predictions of geological, rock mechanical, hydrogeological and hydrochemical conditions along the planned tunnel for the Äspö HRL. During construction of the tunnel geological and hydrogeological mapping were made and comprehensive investigation were performed to get geological, rock mechanical, hydrogeological and hydrochemical conditions which could be compared to the predicted. One objective was to test the ability to obtain a thorough understanding of the rock conditions based on investigations of the surface and investigations in and between bore holes from the surface. By understanding we here mean to obtain sufficient knowledge to show how things are, but also to show how things cannot be. An important part of the comparison of the predictions with the outcome was to evaluate the usefulness and feasibility of pre-investigation methods. This is mainly discussed in an other article. Another purpose was to evaluate the models made. This is discussed in this article.

1 Introduction

The site characterisation work of Äspö has been carried out as an interdisciplinary work in the fields of geology hydrogeology and hydrochemistry. It has been carried out in different steps focusing on different scales simultaneously. The goals of preconstruction and construction phase characterisation 1986 - 1995 were to :

- demonstrate that investigations at the ground surface and in bore holes provide sufficient data on essential safety-related properties of the rock at repository level,
- refine and verify the methods and the technology needed for characterisation of the rock on the detailed site investigations.

The aim was also that the site investigations should give some experience in order to:

- refine and test on a large scale at repository depth methods and models for describing groundwater flow and transport of solutes in rock.
- provide access to rock where methods and technology can be refined and tested so that high quality can be guaranteed in the design, construction and operation of the final repository.

Characterisation of the rock conditions at the Äspö site began in 1986. The first four years were devoted to investigations from ground surface and in bore holes drilled from the surface. Models of rock conditions at depth were developed on the basis of these investigations. The models were evaluated and further detailed during the following five years (1990 - 1995) when the laboratory was constructed. The laboratory tunnels and shafts extend down to a depth of 450 metres below ground level. Data collected in the 3.6 km long tunnel, in surrounding monitored bore holes and in bore holes drilled from the tunnel throughout the construction phase were evaluated and compared with predictions based on the pre-construction models.

2 Approach to test models

The Äspö Project was structured to facilitate testing of the reliability of site characterisation methodology. This included:

- iterative updating to allow for increasing the details of models and possible reinterpretation of previous data sets.
- multi-disciplinary and integrated approach to data collection and interpretation.
- selection of key issues for site characterisation for study and subsequent substructuring in subjects and geometric scales.

The Äspö key issues for site characterisation were Geology, Mechanical stability, Groundwater flow, Groundwater chemistry and Transport of solutes. A basic requirement for modelling of the mechanical stability, the groundwater flow, the chemical conditions and the transport of solutes is a good geological-structural model of the site. Out of the five key issues, most work during 1986-1995 was devoted to the issues Geology, Groundwater flow and Groundwater chemistry.

3 Main concepts

The geological models of Äspö consist of a lithological description and a description of the discontinuities (fractures and fracture zones).

The hydrogeological model comprises the following geometrical concepts: Hydraulic conductor domains (corresponding mainly to major fracture zones. Deterministic feature assumed to have constant properties) and Hydraulic rock mass domains (rock mass outside Hydraulic conductor domains described as a stochastic continuum)

The major processes in the groundwater chemical model are mixing and groundwater/rock interactions. The mixing of different end-members (original groundwater types) is a physical process taking place both at present and in the past. Groundwater/rock interaction includes all processes affecting the groundwater chemistry, specifically calcite saturation, redox and biological processes, which have the greatest influence on the ground-water composition. In Rhen et al /1997c/ the concepts are outlined in more detail.

4 Models based on surface bore holes and surface based investigation methods

During pre-investigations for the Äspö site the analyses of the data were frequently summarised in different kinds of models after each pre-investigation stage. Development of these models is the described in Wikberg et al /1991/. Details of the previous models, the characterisation work and investigation methods are found in Gustafson et al /1988/, Gustafson et al /1989/, Stanfors et al /1991/, Almén and Zellman /1991/ and Wikberg et al /1991/. Predictions made for the construction phase were presented in Gustafson et al /1991/.

5 Characterisation results based on tunnel bore holes and mapping of the tunnel

The predictions in Gustafson et al /1991/ were compared with the characterisation results based on tunnel bore holes and mapping of the tunnel in order to assess the the models made and the pre-investigation methods used. The overview of investigation methods used 1986-1995 is presented in Stanfors et al /1997a/. The detailed evaluation

of the results from the pre-investigation phase is reported in Stanfors et al /1997b/ and Rhén et al /1997a/ and summarised in Rhén et al /1997b/. Üpdated models of Äspö based on site characterisation 1986-1995 are reported in Rhén et al /1997c/.The feasibility and usefulness of site investigation methods are described in Almén et al, /1994/. Some results of the assessment of the models made are presented below.

Lithology

The reliability of the predictions of the relative amount of the main rock units is rather good mostly due to well exposed bedrock and borehole data (core and geophysical logging). The very irregular distribution of rock types like the fine-grained granite and the greenstone makes it almost impossible to describe the position and extent of the minor rock units.

Discontinuities (fractures and fracture zones)

On the site scale is possible to localise sub-vertical major fracture zones (>5 metres wide) during the pre-investigation phase at shallow depths. However, it is very difficult to predict more exactly the position, width and character at increasing depth. The error in predicting the position of a major fracture zone at depth is mainly due to the uncertainty of the dip. There is generally good agreement between the prediction and observations concerning the main orientation of sub-vertical fracture zones and their importance for construction (Figure 4-1).

There is not always a clear correlation between distinct geophysical indications and the real importance of a fracture zone. For example, the topographically and geophysically very distinct regional zone EW-1 - which divides Äspö into two blocks - is of fairly low transmissivity and mostly of rather good mechanical strength for construction purposes. Zone NE-1, however, which was crossed by the tunnel, proved to be very difficult to excavate due to very high transmissivity and low mechanical strength. This zone was rather faintly indicated geophysically during the regional stage of pre-investigations, partly because it is located under the sea.

A number of minor, mostly steeply dipping, fracture zones were predicted to intersect the tunnel volume trending NNW-NNE. On the 500-m site scale, however, no exact position of a particular zone was predicted - only the frequency and main orientation of the zones.

Combined results from tunnel mapping and drilling show the characteristic pattern of the 'NNW structures'. They mostly occur in a complex pattern of steeply dipping fractures (fracture swarms) and some decimetre-wide 'fracture zones' trending WNW to NE. Many of the narrow fracture zones are connected to veins or dikes of fine-grained granite. The character of many of these structures as 'fracture zones' is not very evident. They should rather be described as a 10-30 m wide swarm of mostly subvertical conductive fractures trending WNW-N where the WNW trending fractures are normally the most frequent and hydraulically important.



Figure 4-1. Structural model of the Aspö area, with predicted main structures at ground level, prior to construction (left) and after construction (right).

The discrepancy between the prediction and outcome regarding minor fracture zones shows that it is almost impossible to predict the exact position of a specific minor fracture zone based solely on surface data and information from a single bore hole in or close to an actual rock block. The main orientation, however, of the 'NNW fracture zone system' and its water-bearing character was in fair accordance with the prediction.

As regards predictions of small-scale fracturing on the 5-m scale for typical examples of the four main rock types, there is good agreement between the prediction and outcome regarding 'fracture minerals' and 'main fracture orientation' (especially concerning the two dominant fracture sets striking approximately E-W and N-S) and less good regarding fracture spacing and fracture length.

Hydraulic conductor domains

The types of method and number of hydraulic tests used were mostly sufficient to define the hydraulic conductor domains near the Äspö HRL. However, the hydraulic tests in the core holes were less extensive in the uppermost 100 m of the bore holes and due to this the interpretation became more difficult and uncertain.

Hydraulic rock mass domains

The statistical properties of the hydraulic conductivity of the hydraulic rock mass domains were estimated approximately correctly for southern Äspö with the methods used.

There are, however, a few problems concerning the evaluation of the properties of the hydraulic rock mass domains. It will be a cumbersome task to estimate properties if the rock mass is heterogeneous on a large scale and anisotropic. There is a scale dependency that has been handled using data from a number of bore holes, with tests performed over different lengths in them, to formulate an empirical relationship. Despite the difficulties in estimation of the hydraulic properties, the groundwater flow modelling results are considered good, see Figure 4-2.

Groundwater chemistry

The development of investigation and modelling methods has changed the significance of groundwater chemistry from being solely a question of obtaining a span of realistic variations in groundwater composition to being a description of the episodic and continuous evolution of the hydrochemistry in the past. The present knowledge is a detailed understanding of the hydrological and hydrochemical conditions prevailing since the latest glaciation. At depths of more than 500 m a saline water dominates, see Figure 4-2. At this depth, the water has not been significantly affected by the conditions prevailing since the last glaciation. Glacial melt-water is found at depths of 200 to 300 m. This could have been caused by either as a short pulse, or gradually over much longer time span. There are also minor proportions of glacial water at depths of more than 500 m. At present it is not possible to tell definitely whether this water has a different origin than that of the glacial water at a depth of 200 to 300 m.

Biological activity is the most recent process taken into consideration in the modelling work. At present there is a good picture of the magnitude and the location of the biological processes.

6 What new information was/can obtained from the investigations performed in the tunnel ?

The natural variability of some parameters are quite large and increasing the sample size by sampling in the tunnel made the statistical distributions more reliable. A better 3D description of the fractures was obtained, although the tunnel also sets limits for observable trace lengths. The investigation along the tunnel increased the level of detail in the model. The new data resulted in more precise dips of zones intersecting the tunnel and more data on the hydraulic properties of zones and rock mass.

During the construction work anisotropic conditions of the rock mass were established. These were based on the systematic hydraulic testing along the tunnel ramp, and, as the tunnel was made in a spiral on southern Äspö, the possibility of testing the anisotropy of the rock mass became quite good. The mapping of grouted fractures also gave good indications of fracture sets that were hydraulically active on a local scale. The probe holes used for systematic hydraulic testing along the tunnel were also used for pressure measurements. These measurements give a good picture of the heterogeneous nature of the crystalline rock, shown as a large variability of the pressures close to the tunnel



Figure 4-2. Left: Measured and calculated drawdown during construction. The black bullet shows the position of the tunnel face, the + shows the positions of the bore hole sections for the measured water level. The water table is shown with the tunnel face at chainage 2875 metres (400 metres below the surface) for measured data (top) and Model 90 (middle) and for Recalc 90 (bottom). Recalc 90 is equivalent to Model 90, but with the measured inflow rate and a new deterministic water-bearing zone intersecting the shaft. Right: Classification of groundwaters according to Model 90 and Model 96. Model 96 is based on the combination of statistics and interpretation of water type origin and their mixing proportions. Model 90 is based on multivariate statistics only. A is similar to meteoric water, B does not correspond to glacial water, C corresponds to Baltic sea water and altered marine water and, finally, D corresponds to saline water.

The large number of sampling points in the tunnel has given a more detailed picture of the variability of the groundwater chemistry. The biological activity was not considered in the pre-investigations but has now shown to play an important role in evolution of the groundwater chemistry.

7 What cannot be obtained from the tunnel investigations ?

Excavation of a tunnel causes a large hydraulic impact and it is hardly possible to collect water samples representing the undisturbed conditions, at least in the more conductive

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bedrock. The characterisation of the undisturbed groundwater chemistry conditions must mainly be made during the pre-investigation with a well-designed program to get high-quality water samples.

It is also essential for the hydraulic modelling to have reliable measurement of the undisturbed hydraulic conditions (mainly pressure but also salinity distribution and groundwater fluxes). The data are needed for the calibration of the flow models made but also for interpretation of the hydrochemistry data.

8 Conclusions

The following are the most important conclusions concerning models made:

Geology

- Predictions of lithology on the regional scale are mostly very reliable as regards the distribution of major lithologic domains such as granite diapirs and big massifs of basic rock, where we had aero-geophysical data and well exposed bedrock.
- The main rock types is generally well predicted for most of the tunnel rock volume whereas the spatial distribution of minor rock types is very uncertain.
- The position and general properties of major fracture zones are accurately obtained from the surface and bore hole investigations in particular for subvertical structures. The main structural pattern is normally revealed at an early stage of the pre-investigation phase using airborne geophysics and lineament interpretation (existence and extent of major structures). Accurate information on the dip and character of the structures was obtained from more detailed investigations in the form of ground-based geophysics and drilling. Small scale fracturing was became well described with the tunnel data but it turns out that it is difficult to get a base for characterisation of discontinuities in the scale 10-100 m.
- The regional investigations should be somewhat more extensive for a deep repository than was made for the Äspö HRL. The investigations should also have approximately a constant coverage over the area of interest (regional or site area).

Mechanical stability

- The difference between the results from laboratory testing of rock type parameters in the pre-investigation phase and the excavation phase is significant. The outcome for several parameters were wider than the predicted range, thus not fully accounting for the natural variations in the rock.
- The prediction of rock stress orientation corresponds well to the outcome. The relation between the maximum horizontal stress and the theoretical vertical stress, Ko, was predicted to be in the range of 1.7 while the outcome was 2.9. The difference between the predicted rock stress levels and the outcome can be explained by

geological variations and due to the different methods used to make the measurements.

• The prediction of rock quality for the tunnel, using the RMR system, show acceptable correspondence to the observations made in the tunnel.

Groundwater flow

The hydraulic test methods used can in general be said to be sufficient for the models made.

- To construct a reliable model it is important to perform tests on different scales systematically in the bore holes, both for scale relationships but also to gain flexibility in the interpretation of how to divide the rock mass into hydraulic conductor domains and hydraulic rock mass domains. It is also important to perform large-scale interference tests for modelling purposes.
- For the interpretation of the hydraulic conductor domains it is important to work in close co-operation with the geologists and to have a good three-dimensional CAD system.
- A site that is heterogeneous on a large scale and anisotropic conditions makes the investigations and evaluation work more extensive and difficult. However, this character may only be established after quite extensive investigations.
- It is probable that there is some spatial correlation within the hydraulic rock mass domains due to some large and more transmissive features not accounted for in the present concept used. Efforts should be made to develop a more realistic spatial correlation model for the hydraulic conductivity.
- The groundwater flow models used work satisfactorily in several aspects but developments are still needed concerning spatial correlation models, more efficient handling of input data and calibrations and also to obtain better visualisation of the results.

Groundwater chemistry

- The processes considered to have the largest impact on the groundwater chemistry are mixing, calcite dissolution and precipitation, redox reactions and biological processes. In addition to these fast processes, the long-term groundwater/rock interaction has largely affected the groundwater chemistry and produced a brine with a total salinity of nearly 100 g/l.
- Mixing of water from different sources is considered to be the main reason for the observed hydrochemical situation.
- It has been clearly demonstrated that the groundwaters at depths greater than 100 m are reducing, and that the dissolved oxygen in the infiltrating surface water is consumed by bacteria.

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CHARACTERISATION OF CRYSTALLINE BASEMENT STRUCTURES BASED ON THREE-DIMENSIONAL VISUALISATION OF GEOINFORMATION, SKI SITE-94 AND FOLLOW-UP PROJECTS

Sven A. Tirén GEOSIGMA AB, Box 894, S-751 08 Uppsala, Sweden. (sven.tiren@geosigma.se)

Clifford I. Voss U.S. Geological Survey, 431 National Center, Reston, VA 22092, USA (cvoss@usgs.gov)

Abstract

Studies of a hypothetical repository located at 500 m depth in Precambrian granitoids have been carried out by the Swedish Nuclear Inspectorate (SKI) as a part of their evaluation of high-level radioactive waste repositories in Sweden. The studies are based on data collected by the Swedish Nuclear Fuel and Waste Management Co. (SKB) at their Äspö Hard Rock Laboratory (HRL) on the southeastern coast of Sweden. The study involves two phases of building geological structural models: An early phase based on data collected above-ground prior to the excavation of HRL and a follow-up phase based on data collected below-ground in the HRL tunnels during and after excavation. This paper presents some lessons learned during the earlier surface-data-based geological and structural characterisation of Äspö, the SKI SITE-94 project, and the aims of the subsurface-data-based follow-up project together with some preliminary results.

In the earlier SKI SITE-94 study (1992 to 1996), presented geological and structural models of Äspö were based entirely on surface information and information collected in a large number of boreholes. This is the type of information that would be collected at a site for a potential repository prior to excavation of underground facilities. The regional structural setting of Äspö was studied on two scales: a) A 35 km by 25 km map mainly outlining major structures and large scale rock blocks, and b) A 10 km by 12 km map outlining structures transecting Äspö and borders of the triangular Äspö rock segment (about 1 km² large). A three-dimensional structural model was developed containing fractures and fracture zones in a 2 km by 2 km by 1 km deep block of crystalline basement. Structures assumed to control the groundwater flow and rock stability.

The ongoing follow-up project (1997-) is a new independent study focussed on subsurface data collected during and after the excavation of the tunnels and shafts in the HRL. The general approach to interpretation of the HRL data is that it is a separate study; starting from primary data to construct a new model independent of the earlier models, and the modellling evolves outwards from the HRL tunnel to the surface.

1. Introduction

The Swedish Nuclear Inspectorate (SKI) has conducted an integrated performance assessment study, the SKI SITE-94 project (SKI, 1996), in order to obtain scientific guidance for their review of the forthcoming application from the Swedish Nuclear Waste and Management Co. (SKB) to build a repository for high-level nuclear waste at a depth of about 500 m in crystalline bedrock. Äspö island, the location of the intensively-studied SKB Hard Rock Laboratory (HRL), was chosen as the location of the hypothetical repository in the SITE-94 project. Äspö is a triangular island of about one squarkilometre large located on the southeastern coast of Sweden, about 230 km SSW of Stockholm.

The site-specific Äspö data were assembled during 1987-1990 by SKB through surfacebased characterisation of the bedrock conditions. In the SKI SITE-94 study (1992 to 1996), geological modelling was based entirely on the intensive and spatially complex data sets consisting of surface information and information collected in a large number of boreholes. This is the type of information that would be collected at a site for a potential repository prior to excavation of underground facilities. Geological and structural models of the hypothetical Äspö site were developed (Tirén et al., 1996, Tirén, 1997) based on site-specific data (cf. Stanfors et al., 1991). The regional structural context of the Äspö site was given by a compilation of litterature and the production of structural maps: a) A larger scale map (35 km by 25 km) mainly outlining major structures and large scale rock blocks, and b) A somewhat smaller scale map (10 km by 12 km map) outlining structures transecting Äspö and borders of the triangular Äspö rock segment. The three-dimensional structural model developed (Tirén et al., 1997) comprises fractures and fracture zones in a 2 km by 2 km by 1 km deep block of crystalline basement, that are assumed to control the groundwater flow and rock stability.

The ongoing follow-up project (1997-) is a new independent study focussed on subsurface data collected during and after the excavation of the tunnels and shafts in the HRL. The type of surface-based investigations used to develop the first model, the SKI SITE-94 model, generally indicate the character of the bedrock and form the basis for location and preliminary layout of the hypothetical storage facility. During the subsequent excavation of a real repository, data collection, such as borehole investigations and tunnel mapping, continues. This new data could be used to verify and refine the original model. However, in the present study this approach was not choosen. Instead, the HRL data is used to generate a separate model, independent of earlier SITE-94 model, and the interpretation evolves outwards from the tunnel to the surface. This second model may later be compared with the SITE-94 structural model and other Äspö models (including the SKB model) to determine the value of surface-based data collection versus subsurface-based data collection. Later projects will consider hydrogeology, rock mechanics, and other aspects important for the deep repository performance assessment.

This paper is a combination of lessons learned from the SITE-94 surface-based site characterisation study and a presentation of the aims for and recent results of the on-going follow-up project, focussing on:

Sorting of data and identification of critical parameters. Critical parameters show the limitations of the suitable rock volume for the location of radioactive waste storage.

Surface information. The ground is the only extensive surface that reveals the structural framework in the bedrock. Detailed remote and field studies can give a result that closely resembles the structural configuration at great depth.

Orientation of structures. The configuration of brittle structures, such as fracture zones, often mimic on a local scale the regional structure system and the orientation of fractures outlining the morphology of outcrops. Seismic and radar surveys at the surface and in boreholes also provide oriented or semi-oriented data on structures.

Visualisation. Working in a true three-dimensional space simplifies extrapolation of different types of data between boreholes as well as boreholes and the surface. For example, data analysed by three-dimensions visualization may include maps of topographical relief and detailed geophysical measurements, borehole radar reflectors (expressed as planes), sections of crushed rock in boreholes, and indications of groundwater flow in boreholes and tunnels. Examples of four-dimensional visualization are pressure propagation during multi-borehole pressure tests and structural model correlation with paths of pressure propagation (SKI, 1996). To thoroughly evaluate interpretations in a three-dimensional space a stringent modelling proceedure is needed. Working in true dimensional space, analogue map (vertical and horizontal sections) can be useful in the planning of the modelling as well as during the actual modelling progress.

Restrictions and uncertainties. Restrictions in the modelling need to be given as well as the *accuracy* of the input data and the *uncertainties* in the model.

2. SITE-94 – Lessons learned

2.1. Structural characterisation of an area by remote sensing

The results achieved mainly depend on the following parameters:

Size of the studied area should be related to the structural configuration/pattern in the area, which may appear to be obvious. However, some sets of structures may need larger enclosure than other structures.

Resolution in the data determines the smallest detectable structure. However, a classification that distinguishes between depicted fracture patterns in exposed rock and topographically expressed lineaments is needed. Working with high resolution in the interpretation may, for example, enable characterisation of internal structures within a deformation zone and identification of domains having a general increase in the density of minor fractures.

Interpretation of features is made in two steps: 1) Detailed studies – high resolution, and 2) Generalisation, for example aligned structures are connected and by that indicating the trace of exstensive structures expressed on the final version. Preferably, both the detailed and the generalised maps are presented. When using combinations of data sets (for

example, digital elevation model and airborne geophysics), it is advantageous to compare data rather than interpretations, by overlaying the original maps of data. However, the different data sets also need to be interpreted separately.

Remote sensing studies include both the interpretation of lineaments, and maybe more important, the construction of rock block maps. Furthermore, information on late activation of faults (Cambrium to recent) are indicated by, for example, distortion of soft sediments, ground offset, changes in altitude and tilt of the ground surface, and variation in relief from one rock block to another. Study of geometrical pattern of stuctures at the surface (on all scales: internal pattern in fracture zones, relation between the internal fracture zone pattern and the extremal structural pattern, and the overal structure pattern/system) form the basis for interpretation of structural relationships at depth.

2.2. Surface mapping

The aim of the fracture mapping is generally to identify the geometry of rock blocks and to interpret the most probable geometry of the water transporting paths in the bedrock. An efficient mapping method that fulfils the above objectives has been presented by Tirén (1991). It is based on the assumption that fractures or fracture sets that have the lowest tensile strength determine the morphology of outcrops. Therefore, these fractures most probably define the geometry of the transport paths of the groundwater in the bedrock and also define the geometry of the rock blocks, cf. Figure 2-1.



Figure 2-1 a) Geometry of fractures defining the outcrop morphology (702), b) Geometry of HRL borehole radar reflectors (307). c) Fracture zones in HRL (115). Equal area, lower hemisphere projection. Contouring 1%, 2% and 3%. Circles filled grey are cored boreholes.

2.3. Borehole configuration

Structures do not appear randomly (unsystematic arrangements) in the rock as the fracturing of the rock is dependent on applied stress fields, the pre-existing framework of structures in the rock (inhomogeneities), and the rheological properties of the rock. The degrees of freedom for interpretation of the structural framework in the rock are limited and dependent on the location of boreholes. The uncertainties in the structural model increase with increasing depth, as structures at depth may not be correlatable with any

observed structure at the surface. Some structures have finite extensions; others may be very gently inclined and may outcrop far outside the site; still others may be displaced.

In a structural model of a rock volume, confidence in the existence and location of structures is generally not equal in all parts of the model due to sampling density variations. Furthermore, the ability to detect structures in different parts of the rock volume depends on the method used and the orientation of structures. Uncertainties regarding location of structures and especially existence of volumes of low degree of confidence for detection of structures should therefore be presented separately for each group/set of fracture zones. This type of check can be done by graphic visualisation and may be used as an aid in the design of the drilling programme as well as interpretations of hydraulic measurements.

2.4. Presentation of models

The modelling stage differs from the previous stage of evaluation of data in the respect that it is a synthesis of all available data. Modelling consists of several stages such as handling of data, formulation of approach, construction of the model, and description and visualisation of the model. Handling of data consists, in its turn, of compilation of data, correlation of data and recognition of critical parameters. The modelling approach involves definition of modelling restrictions, methodology, systematics and stringency. The construction of the model is governed by the approach and handling of data. The description of the model presents the approach, the handling of data and the constructed model. The static visualisations of a three-dimensional object should be presented as a succession of images viewed from different directions and should possibly be accompanied with block diagrams and thematical images.

Modelling of the distribution of rock types and the structural framework within an area is a continuous process, which is initiated with the review of the regional geological and structural setting of the area. The models are then generally restricted to maps and vertical cross-sections. Uncertainties in the model should be expressed. In Figures 2-2 through 2-5, some examples of models are shown.

2.5. Water in zones

In the first surface-based model, locations of fractures and fracture zones were hypothesised on the basis of surface and subsurface geological and geophysical information, including borehole radar, resulting in a geological structural model of the site that contains 52 fracture zones. Subsequently, the structural model was evaluated for its ability to describe paths of subsurface fluid flow by spatial comparison of structures with flows entering boreholes (from spinner-meter measurements) and by comparison with pressure-propagation paths during hydraulic interference tests. Although the structural model is based on extensive field information, results of the comparison do not unambiguously confirm the power of the model to describe subsurface hydraulics.



Figure 2-2 Primary structural model of Äspö according to the restrictions given in the SITE-94 project (52 structures).



Figure 2-3 A tentative structural model of Äspö comprising regional structures outlining the Äspö Island and local structures on Äspö (modified version of the Primary structural model). Structures extended to the borders of the model are verified by remote sensing.



Figure 2-4 Structural model of internal structures of the Äspö rock segment.



Figure 2-5 Fracture density of Äspö superimposed on model in Figure 2-3 (contours show number of structures within cells of 100 by 100 m).

3. SITE-94 Follow-up project – structural modelling

This project is a new independent study focussed on data collected underground. The data collection was planned and executed by SKB during the excavation of the ramp, the spiral and the TBM-tunnel (lowest part, excavated by using a tunnel-boring machine, TBM) in the HRL. The HRL data are significantly more extensive and detailed than the surface data (cf. Rehn, 1995) and the investigations cover a smaller rock volume (total length of main tunnel is 3600 m).

A fundamental objective was to create a new model independent of the previous work. The detailed planning of the project took place after three weeks of initial field work at the site. The structural modelling in true 3D consists of five separate parts:

- 1. Modelling of individual fractures for the characterisation of discrete features, such as WNW-ESE striking structures, in the HRL tunnel. Fractures are sorted based on strike, dip and water content.
- 2. Correlation of fracture clusters across the HRL tunnel, using the same data set as in step 1.
- 3. Modelling of fracture zones with emphasis on extensive fractures within and parallel to zones.
- 4. Modelling of structures based on absolute orientations of radar reflectors. Sorting is the same as in step 1 but combined with water bearing fractures and mylonites.
- 5. Compilation of a single model guided by the 4 steps above.

Surface data used to locate the outcropping of structures are geophysical and topographical relief maps illuminated from 8 different directions and a structural interpretation of aerial photos. During the modelling, a stringent record has been kept of structure identities to enable the merging of the separate models. In this way, data and interpretations can be "traced".

Some preliminary results so far are:

- In general, drillholes from the surface are almost perpendicular to holes in the HRL. The borehole configuration affects the sampling, especially where the borehole radar is concerned, Figure 3-1 (cf. Tirén, this volume).
- The dominant direction of water-bearing fractures is WNW-ESE although fracture zones oriented in this direction are scarce. The distribution of the fractures is homogenous and pervasive. This fracture orientation dominates in outcrops.
- There appear to be "dry zones" or domains without water-bearing fracture indications. Figure 3-2 shows an example of such a domain. Since the Äspö rock in general is fractured, a 'dry' domain is, in fact, an anomaly and should be studied.



Figure 3-1 Comparison of direction of radar reflectors recorded from surface and from HRL (left) holes (12 surface and 24 HRL boreholes). Contouring 1%, 2% and 3%. Circles filled with grey are cored boreholes.



Figure 3-2 Example of a "dry zone". All wet fractures along the spiral are shown. Dry zone contains no wet fractures.

4. Concluding remarks

It is not the primary objective of SKI to construct alternative models but to investigate methods of data sampling and treatment, accessibility and quality of data. Furthermore, SKI investigates methods to be used for characterising the bedrock based on the available SKB data. This is done in order to obtain scientific guidance for SKI review of the SKB research and development and of the forthcoming application to locate a repository for high-level radioactive waste. In order to fulfil these SKI needs, it is necessary to critically evaluate the entire process of data handling and modelling, which can best be done by actual attempts at structural and hydrogeological modelling.

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DETAILED SITE CHARACTERIZATION FOR FINAL DISPOSAL OF SPENT FUEL IN FINLAND - CASE STUDY LOVIISA

Pekka Anttila, IVO Power Engineering Ltd. Henry Ahokas, Fintact Oy Calin Cosma and Jukka Keskinen, Vibrometric Oy Heikki Hinkkanen, Posiva Oy Pekka Rouhiainen, PRG-Tec Oy Paula Ruotsalainen, Fintact Oy Antti Öhberg, Saanio & Riekkola Consulting Engineers

Abstract

The spent fuel from the Finnish nuclear power plants will be disposed of in the Finnish bedrock. Posiva Oy is responsible for the site selection programme carried out in accordance with the Governmental decisions. Preliminary site investigations were made in five areas in 1987-1992. Based on the results, three areas, Romuvaara in Kuhmo, Kivetty in Äänekoski and Olkiluoto in Eurajoki, were selected for the detailed site characterization in 1993-2000. The final site will be selected by the end of the year 2000.

The interim reporting of the detailed studies of the three areas was made in 1996. In 1997, the island of Hästholmen, as the host to the Loviisa NPP, was included as a fourth candidate site in the programme for the detailed site investigations. The goal is to characterize this site also in detail by the end of 2000 to attain the same level of knowledge as available from the three other sites. The background information existing from the studies made for the construction of the repository for the low-and intermediate-level wastes will create a good basis to reach the target.

The research programme for the detailed site characterization has mainly been focused on groundwater flow and geochemistry due to their importance in terms of long-term safety of the repository. Equipment and methodology development by Posiva has introduced new tools that provide more accurate data on relevant parameters than the ones used in previous stages of site characterization. The programme also contains studies for additional information of the structural and geological properties of the bedrock towards the depth. Also predictive modelling has been made for evaluating the relevance of the assumptions made. The methods applied in the site characterization have comprised, e.g., geological mapping, deep core drilling, groundwater sampling and analyzing, hydraulic testing and geophysical measurements.

This paper discusses the site characterization work performed at Hästholmen during 1996-1998.

1 Introduction

Posiva Oy, a company jointly owned by Teollisuuden Voima Oy (TVO) and Imatran Voima Oy (IVO), is in charge of research and development regarding disposal of spent nuclear fuel in Finland and, ultimately, of the construction and operation of the repository itself. Posiva is also responsible of the site selection programme carried out in accordance with the Governmental decisions. Preliminary investigations were made at five sites in 1987-1992. Based on the results, three of them, Romuvaara in Kuhmo, Kivetty in Äänekoski and Olkiluoto in Eurajoki were selected for detailed site characterization in 1993-2000. In 1997, the island of Hästholmen, as the host of the Loviisa NPP, was included as a fourth candidate site in the programme for the detailed site investigations. The final site will be selected by the end of 2000.

Interim results of the detailed site characterization studies from Romuvaara, Kivetty and Olkiluoto were summarized in 1996 (Posiva Oy 1996a). After that additional investigations have been continued at each site, but from1997 they have mainly been concentrated at Hästholmen. The goal is to characterize the Loviisa site in detail by the end of 2000 to attain the same level of knowledge as available from the three other sites. The background information existing from the studies made for the construction of the repository for operating waste will create a good basis to reach the target within a quite limeted time.

This paper deals with the site characterization work carried out in Loviisa. At first geological background data from previous studies will be briefly described, as well as the results of the preliminary study performed. Regarding the detailed site characterization most of the methods described are previously applied at the other three study sites. As a part of characterization aiming at consistent description of a site integrating the previous and the new results a 3-D structural model with hydraulic parameters has been established for the basis of the numerical groundwater flow modelling. Also geochemical characteristics and the evolution of the groundwater regime have been studied and reported to be used as basic data in the safety assessment.

2 Characterization of the Loviisa site

2.1 Previous investigations

Geological studies have been performed on the island of Hästholmen since late 1960's and the whole 1970's for the needs of the design and construction of the Loviisa nuclear power plant. Experiences were also gained from the rock construction works, e.g., excavations for foundations and cooling water tunnels. Although those activities extended only to the depth of some 30 metres from the ground surface, indications for favourable conditions also deeper in the granitic bedrock were quite evident regarding the final disposal of low and intermediate-level operating waste.

Site investigations for the repository of the operating waste, the VLJ Repository, were mainly performed in 1980's (Anttila 1988), but a lot of additional information was also gathered during the construction phase of the repository in 1993-1996 (Anttila 1997). The site investigations, e.g., 15 boreholes drilled down to 150-240 metres, were concentrated in the western part of the island, but topographical and structural data was also gained by refraction seismics from the surrounding sea area. Figure 2-1 presents the locations of boreholes and seismic sounding lines on the island of Hästholmen.



Figure 2-1. Location of boreholes and seismic lines at Hästholmen.

The host rock is Precambrian rapakivi granite the age of which is some 1640 Ma. The fracture pattern is nearly cubic, as typical for granitic rocks. The main structural features of the bedrock are the three gently dipping fracture zones. The repository is located between the two uppermost zones at the level of -110 metres.

All relevant data from Hästholmen concerning rock types, fractures, fracture zones, geochemistry, hydraulic conductivities etc. has been compiled, digitized and transferred to Posiva's database. These large amount of background information from previous studies has created a basis for further characterization work of the Loviisa site.

2.2 Preliminary study

The objective of a preliminary study in 1996 was to determine whether the site properties were appropriate for final disposal of spent fuel, as compared to properties of other investigation sites. The preliminary study (Posiva 1996b) was primarily based on existing data and further analysis. In addition to the material described above, data was also gathered from the vicinity of the site, as well as general knowledge about the properties of rapakivi granite. The study also included other factors, for example, fuel transport, infrastructure, labour issues and economical effects.

A structural interpretation of the bedrock was made on the vicinity of the island, within a radius of about 20 km (Kuivamäki et al. 1996). The purpose was to identify the most significant crush zones that would limit the rock volume available for the final disposal around the island. In addition, the structural interpretation was complemented by geological mapping of outcrops within a radius of some 5 km around Hästholmen for studying more carefully different rock types and fracture orientations.

To assess the hydrological conditions, previous test results of hydraulic conductivity and observations on pressure head were gathered and analysed. The knowledge of groundwater chemistry were complemented. The preliminary study included also sorption studies, determination of rock mechanical and thermal properties of the rapakivi granite.

The result of the preliminary study was that the bedrock of Hästholmen is suitable for the final disposal of spent fuel, and a bedrock block, large enough, could be located under the island at the depth of some 500 metres (Posiva 1996). With respect to any further investigations, the most crucial bedrock issues seemed to be the occurrence of horizontal crush zones, chemical quality of groundwater and groundwater flow conditions. For studying these features new deeper boreholes should be drilled to a depth of even one kilometre.

2.3 Detailed site investigations

2.3.1 <u>Geological studies</u>

The investigations have included drilling of five from 800 to 1000 m deep boreholes (HH-KR1-5) with a diam. of 56 mm. The sixth borehole with a diam. of 76 mm will be completed in July this year. The target depth is 600-700 m. 3D rock stress measure-

ments are conducted while drilling.

The objective of the drillings has been to extend the structural model generated earlier during studies of the low- and intermediate-level waste repository deeper into the bedrock, to the planned final disposal depth, to check the properties and extent of the observed horizontal zones, and to examine whether similar subhorizontal zones would also occur deeper in the bedrock. Drillings have also revealed properties of the vertical fractured and crushed zones around the assumed final disposal bedrock section volume, and the salinity of groundwater deeper in the bedrock.

A set of measurements and sampling of flushing water was carried out while drilling. Uranine was used as the label agent in the flushing water. Both the volume and the conductivity of the flushing water and the returning water were recorded as well as the flushing water pressure. Drilling cuttings were removed from the borehole by means of airlift pumping and pumping water from the bottom of the borehole trough the drilling pipes. The deviation of the boreholes has been measured with Reflex-Maxibor and Boremac D2 deviation instruments.

Core samples were phographed and logged at the site. Uniaxial compressive strength, Young's modulus and Poisson's ratio were measured from core samples with a portable tester. The strength and elastic parameters will be confirmed with laboratory tests.

The programme for the detailed site characterization includes systematic mineralogical and petrological studies of the drill cores (e.g. Gehör et al. 1997). The main emphasis is to determine the rock types and their mineral and chemical composition, and to identify low temperature fracture minerals, especially, in sections with a high hydraulic conductivity. The results will be utilized, e.g., in geochemical modelling and assessing the origin of the groundwater. The results show that there are four main types of rapakivi granite.

Calcite, dolomite, Fe hydroxides and clay minerals form the most typical low temperature fracture minerals. Fluorite and Fe sulphides have been met less frequently. Fracture coatings by chlorite and chloritic slickensides occur quite commonly in all depths.

During the preliminary study in 1996 several greisen veins were found on the outcrops of the Hästholmen region. These veins, primarily consisting of quartz, mica and topaz, are commonly associated with hydrothermal tin mineralization. The objective of a more detailed geological mapping of the greisen veins was to determine their mineralization potential. The mapping (Kuivamäki et al. 1997) was concentrated in the near vicinity of Hästholmen, but observations were also made over a larger area in order to get a regional perspective of mineralization potential of the rapakivi granite.

Altogether 19 greisen veins were recorded in the vicinity of Hästholmen, none of them on the island itself, and, in addition, a lot of glacial erratics with greisen mineralization. The analyses indicated that elevated Sn, Zn, Pb and Cu concentrations occur only in a few samples. The conclusion of the study is that the potential for economic mineralization in the Hästholmen area is rather limited.

2.3.2 <u>Geophysical studies</u>

Low-altitude airborne geophysical measurements (Multala & Hautaniemi 1997) aimed at gathering additional data on the occurrence of the different rapakivi granite types on the surface and at offering opportunities for the three-dimensional interpretation of rock type units, based on magnetic field. The survey methods included measurement of the total intensity of the earth's magnetic field, electromagnetic measurement and measurement of the natural gamma radiation.

Line kilometres amounted to some 1000 km. The coverage area of measurements was about 140 km². The line interval used was normally 200 m, but in the immediate surroundings of Hästholmen a closer line interval of 100 m was applied. The interpretation (Paananen & Paulamäki 1998) of the occurrence of different rapakivi phases served as a basis for the compilation of the revised bedrock model.

Electromagnetic frequency sounding was applied to study whether there would be groundwaters of different salinity at the investigation site and to locate any interfaces down to a depth of some 1000 m (Jokinen & Lehtimäki 1997). In addition, the general distribution of electrical conductivity was examined to assess, for instance, suggestions of fracture zones.

From the most prominent indications, resistivity and total salinity (TDS) of groundwater was calculated (Paananen et al. 1998). Calculated apparent TDS-values varied between 1070 - c. 56000 mg/l. From the total of 52 results, 22 can be classified as saline water (TDS > 10000 mg/l), the rest being brackish (TDS 1000 - 10000 mg/l).

Detailed ground radar survey was applied to study fracturing of the rock surface parts and fracture structures (Sutinen 1997). The investigations provided complementary data on the location of fracture zones and on the validity of the current structural model with respect to structures outcropping onto the earth's surface.

The HSP (Horizontal Seismic Profiling) surveys were done on the sea area around Hästholmen on seven lines. From each line 3...6 reflectors were interpreted. The strongest reflectors are dipping gently to NE.

Geophysical borehole investigations concerned salinity of the groundwater, location, properties and directional distribution of fracturing, connections of the fracture zones between the boreholes, and location and direction of the zones in the larger volume of the vicinity of boreholes. Seismic methods were mainly used for the last-mentioned purpose, since the investigation radius of a borehole radar is limited in the environment of saline bedrock groundwater.

Detailed geophysical borehole logging contained the following methods: measurement of fluid resistivity and temperature, the electrical resistivity (short normal, 0.4 m) and the grounding resistance (single-point array), three-arm caliper, sonic full-wave form, the natural gamma radiation, the magnetic susceptibility, and the bedrock density with the radiometric γ - γ technique (Julkunen et al. 1997). The results were used for detailed interpretation of rock mass (Okko et al. 1998). Borehole scanning techniques dipmeter (Siddans et al. 1997) and digital borehole TV (Stråhle 1998), were applied to locate and orientate single fractures and fracture zones penetrated by the boreholes KR1 - KR3. The obtained detailed fracture orientation results were utilized for the structural interpretation of the bedrock and fracture zones (Paananen & Paulamäki 1998; Okko et al. 1998).

The purpose of the Multi-Offset VSP (Vertical Seismic Profiling) surveys were performed to detect fracture zones, lithological contacts and other anomalies in the bedrock and determine their position and orientation.

The surveys were done in boreholes HH-KR1-3. Seven shot points were placed around each borehole, with offsets from 100 m to 500 m.

Two major seismic reflectors were interpreted from HH-KR1 (Figure 2-1). The first intersects the borehole at 530 meters with the dip 77 ° and the dip direction 130°. The second reflector intersects the borehole at the depth section 910-960 m. The dip of the reflector is 20° and the dip direction is 240°. The second reflector has a very complex shape and the position of the reflector has been calculated in several panels, to better visualize the reflecting surface. This reflector can be observed also from HH-KR2 and HH-KR3 VSP data.

2.3.3 <u>Geohydrological studies</u>

Hydraulic head of the groundwater has been monitored at Hästholmen since 1980. Systematic measurements were done at first in open boreholes, but after 1993 also in multilevel piezometers. The main purpose was to define boundary conditions for the groundwater flow modelling for the disposal of low and intermediate-level operating wastes. The results have confirmed the importance of the fracture zones and hydraulically conductive fracture network for the groundwater flow. The role of rock matrix itself seems to be very small.

Hydraulic conductivities were measured in 1980's with a double packer system. In the detailed characterization phase in 1997-98 the measurements have been made by a flowmeter. This device measures groundwater flow into or out from a given borehole section in constant head conditions (Pöllänen et al. 1997). Hydraulic conductivity and head around the borehole can be calculated when the measurements are made with two different heads. Figure 2-2 gives an example where the equipment was moved in the borehole with 10 cm steps with simultaneous measuring of the flow together with single point resistivity. By this means it is possible to locate and characterize most conductive individual fractures. Detailed flow measurements together with borehole TV results were used, e.g., for determining of the cable length corrections and the exact location of groundwater sampling sections. In addition to the flowmeter, the deep boreholes will be measured with a double packer system (HTU) for verifying the results of the flow meter and to get more data, especially, from the sections with low hydraulic conductivity.



View Point: 1500 [deg.] from North; 00 [deg.] from Horizontal Hästholmen KR1 VSP, shot point L2

Figure 2-1. Major VSP-reflectors in the borehole HH-KR1.



Figure 2-2. An example of results from detailed flow measurement, which is based on moving of 1 m measuring section by 10 cm steps along a borehole. A single fracture gives thus one meter wide flow pattern as can be seen on the left side of the figure. Single point resistances measured during flow logging are presented on the right side.
Groundwater flow across a borehole has been measured with the flowmeter. A special packer system guides the flow through the flow sensors. Four inflatable seals between conventional packers divide 2 m long borehole section into four sectors and the direction of flow can thus be measured, too. An example of results is presented in Figure 2-3 where flow across borehole Y20 was measured before the repository tunnel excavation in the year 1993. The highest stabilized crossflow was detected at the depth of 79.5 m. No measurable flow was detected in the saline part of the bedrock i.e. below 100 m. Measurements were repeated after the excavation of the VLJ Repository and the most remarkable change in the flows across the borehole was the increase of flow at the depth of 79.5 m. Measurements in deep boreholes during 1998 have confirmed the assumption that there is no groundwater flow in the saline part of the bedrock. Detectable flow in deep boreholes has not yet been found in fresh water.





Figure 2-3. Groundwater flow measurements in the borehole Y20.

2.3.4 <u>Geochemical studies</u>

Hydrogeochemical characteristics (Snellman and Helenius 1992) of Hästholmen have previously been studied for the VLJ Repository. Recently in 1997-98 water samples have been taken with a new sampling equipment, PAVE (Ruotsalainen et al. 1996; Ruotsalainen & Snellman this volume).

The general view of the groundwaters at Hästholmen (Ruotsalainen & Snellman, this volume) resemble the other coastal site, Olkiluoto (e.g. Pitkänen et al. 1996; Ruotsalainen & Snellman 1996), with reflections of the ancient saline stages of the Baltic Sea and zonation of different bodies of groundwaters from surface-near fresh to deep saline.

The strongest Litorina effects can be seen at the depth of about 100-400 m with the elevated SO₄, Mg, NH₄, B, trace elements and heavy stable isotopes. Salinity increases with increasing depth suggesting enhanced water-rock interaction and longer residence times. The present TDS_{max} of the deep Ca-Na-Cl groundwaters is about 35 g/l.

The effects of the rapakivi bedrock of Hästholmen can be seen in the elevated amounts of He in the dissolved gases, which generally are mostly composed of N_2 , but also of CH₄ and H₂, suggesting reducing conditions. The observed thick layers of iron oxides and iron oxyhydroxides (e.g. Gehör et al. 1997) as well as the high iron contents of the waters are in good agreement with the results of the microbe studies (Haveman et al. 1998), indicating presence of iron reducing microbes in all samples.

2.3.5 Rock mechanical studies

Some rock stress measurements have been performed earlier at Hästholmen at the depth less than 200 m. These measurements give some indications of the existence of high horizontal in situ stresses at Hästholmen.

Core discing phenomenon has been encountered in several sections during the drilling of the five deep boreholes drilled in 1997-98. Sound core sample have been broken into thin discs after drilling in several sections in all boreholes with a diam. of 56 mm. The connection between this phenomenon with the strength properties of rock and with the stress field in the bedrock are being studied as well as its importance with regard to construction of the facilities.

In order to get a better understanding of the rock mass behaviour around the underground repository, rock stress measurements will be carried out between depth levels 300 m and 800 m. Both 2- and 3-dimensional measurement methods (overcoring and hydraulic fracturing) will be used.

3 Site modelling

The structure and groundwater flow modelling of Hästholmen were carried out in 1996 for the safety assessment of the VLJ Repository. The structure model was transferred to Posiva's computer aided geological ROCK-CADTM modelling system. The CAD model

includes both fracture zones and rock types (Lindh et al. 1997). The model covers the whole island and its near vicinity the bottom level being at -1000 metres.

The bedrock model has been served as planning base for the investigations and it will be supplemented with new results available. The updating of the CAD model is under preparation, but preliminary interpretations (Okko et al. 1998) indicate that several gently dipping fracture zones also exist deeper in the bedrock, down to 1000 metres as can be seen in Figure 3-1. The same low lying orientation seems to reflect also in the lithological contacts of different rapakivi types (Paananen & Paulamäki 1998). The new model will be used as basis for the numerical groundwater modelling.



Figure 3-1. An E-W cross section from Hästholmen showing gently dipping fracture zones. Steep fracture zones in east and west are locating in the sea area.

4 Summary

Detailed site characterization of the Loviisa power plant area has been done from the beginning of the year 1997. The aim is to study and classify the site by the same manner as the other three sites- Kivetty, Olkiluoto and Romuvaara- by the end of the year 2000. A quite comprehensive background material was available from previous studies mainly made for the repository of low and intermediate-level operating wastes. These results indicated gently dipping fracture zones, low lying contacts of different types of the rapakivi granite, and increasing salinity with depth. During the two last years the bedrock and groundwater conditions have been studied and characterized down to the depth of 1000 metres applying the same methods which were used at Posiva's other investigation sites.

The investigation programme is underway, as well as interpretations and modelling of the results, but it seems quite evident that the gently dipping fracture zones are the most striking features in the Hästholmen bedrock. These zones are also very crucial with regard to the groundwater flow and locating the facilities in the rock mass. The results of geochemical analyses indicate reducing groundwater conditions and increasing salinity with depth, the maximum TDS is so far about 35 g/l.

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AN OUTLINE OF 1994-1996 GEOLOGICAL STUDIES FOR UNDERGROUND LABORATORY SITING IN THE CHARROUX-CIVRAY SEDIMENT-CAPPED GRANITIC MASSIF-(SOUTHERN VIENNE-POITOU-FRANCE).

Denis VIRLOGEUX

ANDRA, 1-7, rue Jean Monnet, 92298 Châtenay-Malabry, France. Denis.Virlogeux@andra.fr

ABSTRACT

Following the selection of four potentially favourable districts, ANDRA carried out a comprehensive geological investigation in the cantons of Charroux and Civray in order to assess the suitability of a large volume of granitic *s.l.* rocks to host an underground laboratory according to safety regulations.

The variscan basement is a massif of clustered-coalescent Kalkaline-alkaline to subalkaline plutonic bodies ranging from diorite to granodiorite and monzogranite, overlain by about 150m of Jurassic sediments. These plutons have an age of 355 ± 10 My, and were formed concurrently before intrusion of a 320-300 My old leucogranitic pluton.

Surface mapping, regional aeromagnetic and gravimetric surveys, seismic reflection lines and 16 cored boreholes led to the selection of a tonalitic unit near La Chapelle-Bâton as the target formation to be proposed for detailed study. This volume extends over an area of more than 3 x 4km at the surface and at least 800m vertically. There appears to be no prohibitive factors to installation of an underground laboratory for further exploration, particularly from the hydrogeological standpoint :

- This sector avoids the most complex part of the massif and is located far enough from the Availles-limouzine crustal-regional fault and the Asnois-Rochemeaux fault. It is located in a region where the topography, generally very flat, produces low hydraulic gradients and, as a result, weak impetus to deep hydrogeological circulations.
- The area, and intrusive bodies of this type, offer no possibility of economical natural resources.
- Magmatic joint-type small fracturing shows no variation with depth and polyphasic hydrothermal history has led to plugging the fractures with clays and carbonates. Alkaline fluids crystallising Adular (-126 My) has led to a strong reduction in the initial permeability of basement paleo-weathering zone.

The horizontal and relatively fault-free sedimentary cover reveals a simple tectonic history during the last 200 My. One of the objectives of the laboratory study program will be to confirm the conceptual model of slow, shallow circulation in depth, based on the following data :

- Low frequency water inflows, obtained in the boreholes by pumping and testing, show the very low permeability of (pluri)hectometric blocks $(1 \times 10^{-10} \text{ to } 4 \times 10^{-13} \text{ m/s})$ delineated by conducting faults (transmissivity : $10^{-6} \text{ m}^2/\text{s}$).
- Low hydraulic gradients recorded in the boreholes are consistent with regional topography, and hydraulic heads in the granite similar or lower than those recorded in the overlying sedimentary aquifers.

• The chemical composition of « granitic » waters exhibits significant salinity at depth (10g/l), and is different from the Lias and Dogger aquifer waters, indicating limited hydraulic relationships. The origin and age of the salinity is still under debate, even though Br/Cl ratios and several isotopic compositions point towards a marine-sedimentary origin. Salinity and deuterium excess probably implies a within granite residence time of 10⁵-10⁶ year or more for these waters.

Safety scenarios take account of a potential exploitation of the overlying aquifers: influences at depth will depend on the connectivity of the fractures in the granite, and between the granite and the lower aquifer. Underground laboratory will attempt to demonstrate this probable weak connectivity.

Seismicity of moderate but constant intensity on a historical scale must be taken into account in underground experiments.

A 450m depth three branch star-like underground architecture has been chosen to conduct experiments in order to refine the disposal concept to be submitted in 2006.

1. Introduction

Pursuant to the *law of 30 December 1991* relating to the management of long-lived radioactive waste, the French government authorised the ANDRA to conduct preliminary surveys in four departments (Gard, Haute-Marne, Meuse, Vienne) in early 1994. The aim of these surveys was to demonstrate the favourable character of selected geological formations considered as suitable sites for siting of underground research laboratories.

Sites were assessed by reference to a safety regulation (RFS.III.2.f) issued by the Nuclear Installations Safety Directorate. This assessment addressed essential requirements for geological stability and hydrogeology (low permeability, hydraulic heads and regional gradients) and important requirements for mechanical, thermal and geochemical properties and the lack of natural resources. The information obtained during site specific study programmes led to applications in 1996 to build underground laboratories on three sites. They were examined in 1997 (public inquiries, local officials, National Evaluation Commission). Governmental decisions to inaugurate the sites are expected in the course of 1998.

2. Geographic features and regional geology (Figure 2.1 a)

The cantons selected for study in the Vienne, Civray and Charroux, are located in the *Seuil du Poitou* (Poitou-threshold), a 50km-wide path at low altitude (120-160m), linking the plains of the Parisian and Aquitanian Basins. They cover the drainage divide between the watersheds of the Loire and Charente rivers. The physiography is very flat with a highly damaged bocage-landscape. The *Seuil du Poitou* is characterised by a thin layer (\leq 180m) of Jurassic and Tertiary sediments separating two Variscan Orogen-districts : the *Vendée* (Armorican Massif) and the *Confolentais* (Central Massif).

The Vendée consists of contrasting epizonal to catazonal NW-SE units separated by branches of the South Armorican Shear Zone. The site-equivalent is the NE Haut Bocage : a middle to high grade-barrovian unit (Middle/Upper Devonian) with Kalk-alkaline synkinematic mafic intrusions intruded by numerous Namuro-Westphalian peraluminous plutons during the S.A.S.Z. ductile shearing.

The *Confolentais* district is the result of two stages (Rolin and Colchen 1995, Stussi 1995): (1) Barrovian metamorphism with Upper Devonian-Lower Carboniferous late to post-collisional intrusions (sub-coeval Kalk-alkaline, subalkaline and peraluminous granitoïds); (2) Upper Carboniferous un-deformed plutons followed by cataclastic NW-SE dextral transcurrent faults.

The Mesozoic history of the Seuil du Poitou (Gabilly et al., 1985 etc.) began with Permo-Trias continental weathering and peneplenation. Marine transgression occurred during the Hettangian-Sinemurian (clays and dolomites), followed by deposition of Pliensbachian limestones. After the Toarcian marls, sedimentation returns to Dogger platform-limestones. During the entire Jurassic period, the area was a strait between two deep subsiding basins. A Lower Cretaceous-emersion and karstification took place before a short transgressive Upper Cretaceous episode. Final emersion led to deposition of oxidised clays and lacustrine limestone during the Cenozoïc.

3. Geological investigations from 1994 to 1996

Table 2-1	Field	operations	and	reporting	1994-1996
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	Field operations and reporting	Main objectives			
	Teledetection studies and surface mapping Gravimetry-450km ² ; 4020 stations	Fault detection, stratigraphy and structural framework General structure of the granitic basement			
1994	Surface hydrogeological inventory	Surface hydrology and sedimentary aquifers			
	Reflexion/refraction shooting test	Basement paleosurface			
	11 vertical core drillholes :				
	300m mean depth except CHA103 and 106 (600m)	5km net geological and hydrogeological characterisation of the granitic massif.			
	February 1995 : GOVERNMENT REPORTING	CHOICE OF SECTOR East of La Chapelle- Bâton			
	1994-1995 aeromagnetic reprocessing and interpretation (7000km2, 20500km lines)	Regional structural and lithological mapping of the basement under cover			
	2D reflexion shooting : 5 lines, 35.5725km, 4748 points,	Structure of the sedimentary cover and basement paleosurface			
	21 VT destructive 30m drillholes				
1995	4 vertical core drillholes :	2km net geological and.			
	CHA112(579m); CHA113 (300m); CHA115 (302m); CHA117 (399m)	hydrogeological characterisation of the granitic massif.			
	Specific hydrogeological tests CHA106	Granite hydraulic head			
	Wells and springs hydraulic heads reporting	Characterisation of surface aquifers			
	3 piezometric drillholes : CIV202 (158m); CHA205 (167m); CHA206 (140m)	Characterisation of infratoarcian aquifer			
1995 1996	/ Inclined deep cored drillhole CHA212 (996m)	Characterisation on the proposed laboratory site.			
	2 shorts cored drillholes CHA118 and CHA119 (Tertiary+Dogger)	Sedimentary cover geotechnical characterisation on shafts sites			
1996	Hydrogeological drilhole CHA312 (192m)	Hydrogeological characterisation of the basement paleosurface			
	Hydrogeological tests CHA212/112	and of the granite on laboratory site.			
	Hydrogeological reporting (simple and multipacker completions)	Characterisation of surface aquifers and granite in depth (pressure-temperature)			

4. Geology of the Charroux-Civray granitic massif (Figure 2.1 b, c)

The Charroux-Civray massif is mainly composed of Kalk-alkaline and sub-alkaline clustered and synchronous plutonic bodies. They show frequent mingling processes and belong to the late-Devonian Limousin Tonalitic Line (Gagny and Cuney, 1997). Kalk-alkaline facies (~49%-gabbros-diorites to biotite-granites) show predominant tonalites occurring in multiple but homogeneous injections. Mg-K subalkaline facies (~39%) are monzogabbros, quartz-monzodiorites and monzogranites. U/Pb dating (Bertrand *et al.*,1997) attribute -365 to -345 My ages (syn/post-collisional) to both trends. Peraluminous leucogranitic facies (~21%) are Namuro-Westphalian. Some microgranite (310-315 My?) and dolerites/lamprophyres (295 My) veins represent the last Variscan stages.

Hydrothermal alterations have led to a strong plugging of joints and (dam) fractures with clays and carbonates. The two main stages (Cathelineau *et al.*1997) are : (1)Variscan veins with Quartz + Chlorite \pm Epidote \pm Prehnite etc. (130-350°C); (2)Mesozoïc veins with Carbonate + Adular \pm Quartz \pm Fluorite etc. (75-110°C) and late Calcite + Baryte or Kaolinite (<50°C). The first Mesozoïc brines are probably related to the Atlantic/Gascoyne-Gulf rifting as well as the alkaline flows across the weathered paleosurface-zone crystallising Adular (-126 My by K/Ar dating). This also led to a strong reduction of the initial permeability.

A negative gravimetric anomaly (>-20 mGal) of the capped basement has been observed by the 1995 survey. A gravimetric/magnetic modelling (Figure4-1) describes the massif in depth (Virlogeux et al. 1997) :



Figure 4-1 2.5D crosssection of gravimetric/magnetic modelling of the site

(1) the vertical geometry and deep roots of the L.T.L granitoïds intruded by a large batholith of leucogranite (roof >-1.5km with little apophysis), (2) the crustal features of the *Availles Limouzine* cataclastic zone. The aeromagnetic data show that the L.T.L plutons belong to the largest group of this type in France, located between two transcurrent crustal regional faults : the NW-SE *Availles-Limouzine* fault (brittle) and the NNW-SSE *Parthenay-Ruffec* fault (ductile-brittle).

The 150m thick sediment cap could be considered as a major handicap for site studies, but it reveals recent tectonic events and gives precious information concerning site stability. The main faults crosscutting the cover around the site are : (1) NW-SE regional faults ; the crustal scale *Availles-Limouzine fault* and the more secondary *Asnois* fault, (2) NS local faults on both side of the lab-site. Except for the *Availles-Limouzine* fault where Pyrenean movements are known, the tertiary sediments overlap the other faults on the site. The proposed laboratory site is a 3x4 km surface far from these faults. Seismic reflection survey confirms the lack of faults with a significant vertical throw on this site.

The mean linear density of (even <1mm thick) fractures is approximately 4 per meter and their multi-scale organisation (Cassard *et al* 1997) shows that 90% are <5 mm thick and related to decimetric-decametric extensions. These little joints, almost systematically sealed, belong to the early magmatic system in close connection with the magmatic foliation (Gagny, 1997). Orientations show a great dispersion (WNW-ESE, NW-SE, NS, NE-SW maxima) and a mean 60°W dip. Latest shears occurred (20%) without inducing new fractures. (Multi)hectometric faults with gouges (>200 mm thick), divide the granitic volume into major blocks. Cores and BHTV images have helped in building a determinist model of these fractures.

5. Hydrogeological and hydrogeochemical characterisation

As a consequence of the great difference of salinity between sedimentary aquifers and deep granite-waters, water-conducting fractures could be located using electric conductivity and thermometric logging (Seguin and Squarcioni, 1997). The very low water-production made classical flow-logging while pumping useless.

In 1994, global tests and logging show that producing zones were thick (dm-m) and cataclastic. Maximum transmissivity around $10^{-6} \text{ m}^2/\text{s}$ was almost constant in all drillholes. In 1995, the same tests show the lowest density of conducting faults East of the Chapelle-Bâton In 1996, tests and measurements were conducted on the pair of wells CHA112/CHA212 located on the proposed lab-site. The inclined (1000m) CHA212 oriented along the minimum of fracture-azimuths optimised cross-checking of fractures. A neighbouring hole (CHA312) targeted the sediment-granite interface. Tests between packers showed very low permeability-blocks bounded by (pluri)hectometric conducting faults. In CHA112, one fault near the paleosurface, of $10^{-6} \text{ m}^2/\text{s}$ (transmissivity per m $\sim 10^{-7} \text{ m/s}$); in CHA212, three faults of 10^{-10} to 10^{-8} m/s. Permeability's in the blocks are between 10^{-14} m/s and 10^{-10} m/s (hydrothermal plugging). Diffusion-coefficients (Tritium-water) range from $10^{-14} \text{ m}^2/\text{s}$ (« fresh »), 10^{-13} to $10^{-12} \text{ m}^2/\text{s}$ (hydrothermalised), to $10^{-10} \text{ m}^2/\text{s}$ (fault-boundary) (Tevissen, 1997).

The granite is overlain by two aquifers separated by Toarcian marls : (1) the upper Dogger-karst free aquifer and (2) the lower Infra-Lias confined aquifer. The latter is strongly depleted during irrigation-periods. In the laboratory sector, pressure recordings (1996-1997) measured between multipacker well completions (CHA106-112) in the granite show no variations with those sharp seasonal variations. It does not demonstrate a total absence of hydraulic relations but it is an indication for the lack of a simple and direct connection. Outside the sector, variations can be significant (i.e. CHA102 close to *Asnois* fault). Safety scenarios take account of a potential exploitation in the overlying aquifers : effects at depth will depend on the connectivity of fractures in the granite and between the granite and the cover. One of the objectives of the underground laboratory will be to attempt to demonstrate this probable weak connectivity.

Results of a limited number of granite water samples (Matray et al., 1997) show an increasing salinity, from a >1 g/l-HCO₃-Na-SO₄- (200m depth) to a 10 g/l-Na-Cl (350m depth); distinct from Dogger-water (Ca-HCO₃-N) and Lower Lias-water (Ca-Na- HCO₃, F). In a $\delta^2 H/\delta^{18}$ O diagram, deep granite-waters show a ²H-excess clearly distinct from cover and upper granite-waters fitting the world meteoric line. The origin of the salinity has been assessed (Cathelineau et al.; Savoye et al., 1997): chloride-leaching from granite (fluid inclusions, minerals) is considered unlikely, but the contribution of fracture-carbonates and microporosity is possible. Br/Cl, as well as B, Sr and S isotopes (Michelot et al., 1997), support a marine or evaporite-dissolution origin (mesozoïc?). First results show a secular equilibrium between ³⁶Cl-content and neutronflux from granite suggesting a minimum 1-1.5 My for salt seeping. The age of water s.s. is unknown but ²H-excess could be generated by low temperature fractionation (silicate hydrolysis and phyllites crystallisation) over a minimum residence-time of 10^5 to 10⁶ years (Michelot et al., 1997). These preliminary geochemical results lend support to the conceptual model of a slow and limited horizontal hydraulic flows in the granite deep under the cover.

6. Geological stability

There is no evidence of neo-tectonic movements. Modelling the Paleogen continental surface (Wyns, 1997) shows that its total vertical deformation is related to a regional scale (>50 km); local deformation is weak, within the error-margin. Local movements are older than 20My, related to the Pyrenean phase and Oligocen rifting. Seismicity is moderate, but significant, and of constant intensity (historical scale). A VI MSK-seismic event occurred in the area in 1901, and the Asnois or other NW-SE faults to the south should be considered as seismogenic. No seismic events having magnitudes exceeding 4.0 have been recorded 30 km around *Charroux-Civray* over the last 30 years.

7. Conclusion : the underground research-laboratory.

The 1994-1996 investigations led to the choice of a tonalitic volume well removed from pluri-kilometric faults. It shows no prohibitive factors to installation of an underground laboratory for further exploration; e.g. low hydraulic gradients and absence of economic resources. Underground laboratory studies are now necessary to specify the characteristics and role of the hectometric scale conducting faults, and the sizes and distribution of low-permeability blocks. A three branch, star-like architecture of galleries (120°) at 450m depth has been proposed for the laboratory. The branch orientations take into account the main directions of faults. The W branch is designed to observe the evolution of fracturing towards *La Chapelle-Bâton* local fault, the other branches are oriented towards the transition to other facies (NE monzodiorite, SE monzogranite).

8. Aknowledgements

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Important achievements from the integrated site investigation of Äspö

Peter Wikberg Ingvar Rhén Roy Stanfors SKB VBB-VIAK RS-Consulting

Abstract

The site characterisation for the Äspö Hard Rock Laboratory started with a comprehensive investigation programme including drilling of 15 deep core drilled holes to a maximum of 1000 m and twenty shallow percussion holes to a depth of 100-150 m. These investigations were carried out in different stages and focusing on different scales, starting from the regional scale surrounding the Äspö island and ending with the detailed descriptions of the rock volume where the tunnel was to be constructed.

During construction the tunnel was mapped and probing holes were drilled into the rock ahead of the tunnel front. Data from these bore holes were used to detail and update the models from pre-investigations, especially regarding the smaller scale in between the major water conducting fracture zones which were not possible to describe on the basis of surface bore hole investigations.

The planning of the bore hole campaigns and the modelling of the results from each investigation batch was made in common for geology, hydrogeology and hydrochemistry. This made it necessary to constrain each of the individual models to fit also the other disciplines. The common bore hole approach made it possible to plan the investigations in a way to minimise disturbances and to take advantage of combined hydrochemical sampling and hydraulic pumping tests.

Experiences showed that the hydrochemical conditions are even more easily disturbed than expected. A modified methodology for hydrochemical sampling will be developed. Quality classification of the hydrochemical data and defined programs for analyses were developed during the tunnel construction phase and will be useful for the future. Microbiology was also found to make important contributions to the evolution of the hydrochemistry and will be further investigated.

Major fracture zones and the average amount of the main rock types defined were adequately predicted with the pre-investigation methods used. The spatial distribution of minor rock types along the tunnel was not possible to predict due to the heterogeneity of the rock mass. The frequency of minor fracture zones was correctly predicted but the spatial distribution along the tunnel was not possible to predict.

The hydrogeological methods used was mainly sufficient for the models made. It is however important to perform tests on different scales systematically in the bore holes, both for scale relationships of the hydraulic properties but also to gain flexibility in the interpretation of how divide the rock mass into sub volumes with different hydraulic character.

INTRODUCTION

Site investigations were carried out at the island of Äspö and its surroundings, starting from the end of 1986 and ending in 1995. During this almost ten year period different properties of the bedrock was examined and tested. The investigation work was carried out integrating the disciplines of geology, geohydrology and hydrochemistry. Planning of the field work was done by a core group of principal investigators for these disciplines and the Äspö project manager, see Bäckblom /1998/ and /Rhe'n et. al, 1998a/. Each of the principal investigators was responsible for the quality of the collected data and the interpretation of the data. At the end of each investigation stage the principal investigators made an interdisciplinary reporting of results and models.

PRE-INVESTIGATION STRATEGY

The first stage goal of the Äspö project was to verify the pre-investigation methods to be used for the spent fuel repository. The first part of this work was to plan the Äspö site investigation programme as an interdisciplinary work to be carried out in stages. The amount of work, i.e. number of boreholes needed, was decided gradually as the work was progressing. The work was focussed on selected key issues and geographic scales

Out of the five key issues, most work during 1986-1995 was devoted to the issues Geology, Groundwater flow and Groundwater chemistry. Mechanical stability addressed issues relating to excavation stability during construction of the laboratory. Transport of solutes included investigations of fracture connectivity, transient flow of natural isotopes and assessment of flow porosity. Some important achievments for each key issue are presented below. The entire evaluation work is presented in /Rhén et.al, 1997a, Rhén et.al, 1997b, Rhén et.al, 1997c, Stanfors et.al, 1997 and Ahlmen et.al, 1994/.

GEOLOGY

Modelling

A basic requirement for meeting the needs of repository engineering and performance assessment is development of a good geological-structural model of the site. This has been achieved in the quite complex geological environment at Äspö.

The geological-structural model is the simplified description of the lithology and fracturing. The simplification of the geological medium to a structural model is one of the most crucial issues in site characterization as this simplification provides the basis for design and modelling work for the other four site characterization key issues. A description of the lithology and main discontinuities is needed to provide a framework for all modelling work concerning mechanical stability, groundwater flow and groundwater chemistry.

At Äspö the lithology has been classified into the rock types Småland (Ävrö) granite, Äspö diorite, fine-grained granite and greenstone.

There is a special need for a good description of the main structural pattern in a rock mass. Basic elements in a structural model are first of all a good interpretation of the major discontinuities (fracture zones) with respect to position, orientation and character. The identification and description of the fracture zones which are important hydraulic conductors and important for the rock stability were of special interest at Äspö. The discontinuities were classified into major fracture zones (width > 5 metres), minor fracture zones (width < 5 metres), single water conducting fractures and small-scale fractures.

The comparison between predictions and tunnel data shows that most of the predictions for major subvertical fracture zones (> 5 m wide) were reliable both with respect to existence, geometry (*Figure 1*) and geological character.





In addition to the major fracture zones, Äspö is intersected by a number of narrow, steeply dipping transmissive fractures or minor fracture zones trending WNW-NNW. The existence of minor fracture zones was predicted and their existence has been confirmed. The existence and frequency of these zones were recognized during the pre-investigation phase but it was not possible to predict deterministically their locations at depth.

Methods

In general the site investigation methods used were adequate for relevant

modelling of the most important parameters needed for construction of the Äspö HRL.

Aerogeophysical investigations, gravimetric measurement and lineament interpretation are very useful for the structural-geological modelling work of major structures on a regional scale.

Geological mapping and detailed ground geophysical profiling (electrical and seismic refraction investigations) indicated minor structures in the site description stage. Borehole investigations (core logging and geophysical logging) provided important data for the characterization of the rock mass at depth. Determination of fracture zone (fracture) orientation was performed by use of borehole radar and borehole TV.

Reflection seismic indications did not correspond to any subhorizontal zones of importance down to 500 m depth. Today both the borehole radar and reflection seismics technique have been developed and probably give better possibilities of detecting subhorizontal fracture zones compared to a few years ago.

There is a need for further development of drilling methodology. It is generally very difficult to penetrate sections of crushed and clay-altered rock using small bits without grouting. To be able to characterize the most fractured parts of a zone a triple-bar coring technique must be used.

Fracture orientation in boreholes was not very successful due to the methods available. Development of digital down-the-hole TV equipment is now a preferred method to verify features mapped in the core with an image of their undisturbed intercept with the borehole. BIP images are also helpful tools in controlling core orientation during mapping.

MECHANICAL STABILITY

Modelling

Rock stress and rock strength are important properties in the engineering of a repository. At Äspö studies were mostly made to find and evaluate potential problems for the construction.

No indications of spalling or rock burst were found and thus the overall expert judgement of mechanical stability at Äspö proved to be correct. The basis for the judgement relied very much on empirical observations in Sweden and elsewhere. The scientific basis for these judgements is limited due to scarce and scattered data, and model and parameter uncertainty. Models for excavation stability have not been thoroughly tested due to the limited stress levels at Äspö.

Methods

During the site investigation, stress measurements were made in three surface boreholes. Hydraulic fracturing was used in two boreholes and the overcoring method in one borehole. Concurrent with the excavation overcoring measurements were made in boreholes drilled from the ramp with the main objective of evaluating the predictions made prior to excavation. The difference between the predicted rock stress levels and the outcome is probably due to the different methods used to make the measurements. The mechanical characteristics were defined by uniaxial compressive tests on core samples. The specimens were prepared before testing and the tests were carried out in a press with very great stiffness.

Core drilling and core mapping provided information for characterization of rock quality. The holes were drilled in different orientations to obtain information on different fracture sets, e.g. steep or subhorizontal. The cores were logged to provide further information on the distribution on different rock types and to determine their fracture frequencies (RQD), fracture distance and fracture surface properties (JRC, JCS and fracture fillings).

The methods used (except for surface properties) for testing were relevant and provided sufficient data for construction purposes.

GROUNDWATER FLOW

Modelling

It is important to determine the existence, geometry and properties of major water conducting features in order to be able to select a repository volume that provides and supports protection of the engineered barriers and isolation of the waste.

The work at Äspö shows that the major factors of importance for modelling the stationary flow system were identified and characterized prior to construction. The major water-conducting features (*hydraulic conductor domains*, consisting of major fracture zones and some of the minor fracture zones (fracture swarms)) were treated deterministically with respect to existence, geometry and properties. The rock mass between the fracture zones was treated as a stochastic continuum and divided into subvolumes (*hydraulic rock mass domains*). The assignment of hydraulic properties to the rock mass was reliable, even if problems exist concerning understanding of scale dependency and anisotropy of hydraulic conductivity.

At Äspö all major fracture zones near or intersecting the tunnel were identified, see *Figure 2*. Most of them, but not all, were found to be highly or relatively highly transmissive (T> 10^{-5} m²/s). The transmissivity can be predicted if there are a few boreholes that intersect a major hydraulically conductive feature where hydraulic tests have been performed in these boreholes.



Figure 2. Left: Model 1990 of hydraulic conductors from the preinvestigation phase - site scale. Right: 1996 model of hydraulic conductors - site scale.

It was also shown that some minor fracture zones (fracture swarms) are highly water conducting and that it is difficult to describe their position and extent precisely in space.

The hydraulic tests performed in a large number of probe holes drilled along the tunnel spiral during the construction showed that anisotropic conditions are present, with the largest conductivity within a sector being WNW to N-S. If the rock mass is hydraulically anisotropic the evaluated properties will, to some extent, be dependent on the borehole direction. It is therefore important to obtain some indication of anisotropy early in an investigation programme for planning the main part of the investigations and also for the evaluation of data.

Methods

The hydraulic test-methods used are in general considered to be sufficient for the models made. Minor problems are that the results are to some extent dependent of the equipment used and thus method developments during a project can possibly affect the results to some extent. It is also difficult to obtain reliable results from low conductivity sections of a borehole because of the elasticity of the equipment and also because of pressure oscillations.

It is important to perform transient hydraulic tests at different scales systematically

in the boreholes both for scale relationships but also for flexibility in interpreting how to divide the rock mass into hydraulic conductor domains and hydraulic rock mass domains. It is also important to perform larger-scale interference tests both for defining hydraulic conductor domains and for calibrating and testing numerical groundwater models.

Flow-meter logging is a fast and useful method for finding major hydraulic conducting features in a borehole and to obtain a rough estimate of their transmissivities. However, in boreholes where there is a high transmissivity feature high up in the borehole and water with high salinity at the bottom of the borehole, flow-meter logging may give erroneous results in the lower part of the borehole. The possibilities of defining low-transmissivity features with the test methodology used are also limited.

There are several difficulties in estimating the proper fluxes in the rock mass from dilution measurements. The technique can be improved, but there are conceptual uncertainties of the coupling between the flow in the rock mass and in the borehole that are difficult to resolve. The dilution measurements, however, are a useful and feasible way of finding out whether or not there are hydraulic communication in terms of flows and not just pressure responses.

The monitoring of the water pressures is judged to have been made with sufficient intensity in space and time. However, it would have been preferable to have had somewhat more measurements of the natural conditions. Due to the large drawdowns close to the tunnel spiral some borehole sections close to the tunnel spiral stopped functioning as the equipment for monitoring the pressure in the boreholes was not designed for these large drawdowns that occurred. It is, however, judged that these two problems did not have a major detrimental impact on the possibilities of evaluating the hydraulic properties and testing the groundwater flow models.

The estimates of the absolute pressures along the boreholes at natural (undisturbed) conditions were useful for the interpretation of the water chemical sampling. However, the measurement technique should be improved to increase the reliability of the pressure measurements.

GROUNDWATER CHEMISTRY

Modelling

The work at Äspö has given a broad understanding of the (chemical) processes that have been active in the past and are currently active in the Äspö groundwater and rock mass. These processes are expected to be typical of a coastal granitic rock environment in Sweden. The processes considered to have the largest impact on the groundwater chemistry are mixing, calcite dissolution and precipitation, redox reactions and biological processes. In addition to these fast processes, the long-term groundwater/rock interaction has largely affected the groundwater chemistry and produced a brine with a total salinity of nearly 100 g/l. Mixing of water from different sources is considered to be the main reason for the observed hydrochemical situation. A good overview of the distribution of the major constituents (main ions) in the water-conducting fractures was achieved already during the pre-investigation phase.

Methods

Most important for investigating the chemical composition of the groundwater in major fracture zones has been the chemical characterization of the ground-water using a mobile field laboratory with the down-hole Eh and pH measuring devices. The second most useful method is the sampling during the hydraulic interference pumping tests. Sampling in shallow percussion boreholes gave useful results.

Sampling of water conducting sections should be undertaken at an early stage in the drilling phase. This was tried at Äspö, but the results were of limited value, since the amounts of drilling water which remained in the samples were too large, primarily, due to the large length of the sampled sections. A better sampling procedure has now been developed to characterize the initial undisturbed situation.

During the tunnel construction phase, groundwater samples were collected through the probe holes drilled into the tunnel walls a few metres back from the front. No special equipment was used for the sampling. Also due to the location of the boreholes it was not possible, nor necessary, to install any permanent sampling devices.

The need for hydrochemical data can be grouped into three categories:

- Reliable data on safety related parameters such as pH, Eh, redox and pHsensitive constituents, (like bicarbonate, iron and sulphide and radionuclide analogous) are needed as input to the safety assessment calculations.
- Chemical processes which determine the present-day situation but also the evolution of the hydrochemistry into the future. Major and minor constituents and end members for different water types are essential in order to understand present-day conditions and useful for the prediction of future conditions.
- To assess the groundwater residence time, there is a need to analyse for stable and radiogenic isotopes as well as for conservative constituents.

The listed sets of data are in some cases extremely sensitive to disturbance while others are fairly robust. Based on the experience obtained from the SKB's early study site investigations in 1982-1984, the Finnsjön project, and in 1986-1995, the Äspö project, the groundwater samples are classified into five different levels with different complexity in sampling and analyses.

Class 1: Simple sampling, basic control of water type; Electric conductivity, pH, uranine*

Class 2: Simple sampling, control of water type;- Electric conductivity, pH, Cl, HCO₃, uranine^{*}. Optional: deuterium, tritium and oxygen-18, Freeze stored back-up sample

Class 3: Simple sampling, determination of non redox-sensitive major comomponents; Electric conductivity, pH, Cl, HCO₃, SO₄, Br, uranine*, major cations (except for Fe, Mn)** and SO₄ as Sulphur on ICP-AES. Optional:

deuterium, tritium, oxygen-18, Freeze stored back-up sample

Class 4: Extensive sampling, complete chemical characterization; Electric conductivity, pH, Cl, HCO₃, SO₄, Br, Fe (total, ferrous), uranine*, DOC, major cations** and SO₄ as sulphur by ICP-AES, deuterium, tritium, oxygen-18, Freeze stored back-up sample, preserved and non-preserved. Optional: HS, NH₄

Class 5: Extensive sampling, complete chemical characterization including special analyses; Class 4 and HS, NH₄. Optional: , NO₃ /NO₂, PO₄, F, I, TOC (like DOC but filtered water sample), Carbon isotopes: ¹⁴C-age, PMC (Percent Modern Carbon), ¹³C per mille PDB (Peedee Belemnite, a standard), U and Th (elements and / or isotopes), other trace elements (INAA and / or ICP-MS), Ra-226, Ra-228 and Rn-222 isotopes

The samplings for the determinations, listed below, should if possible be carried out in connection with a class 5 sampling occasion.

- a) colloids/particles
- b) fulvic and humic acids
- c) gas
- d) bacterial activity
- e) S and Sr isotopes etc.

*) Only measured where uranine was used in the drilling procedure and as long as no extra uranine has been added to the borehole e.g. in tracer tests.

**) Major cations are Na, K, Ca, Mg, Si, Fe, Mn, Li and Sr

TRANSPORT OF SOLUTES

Studies of the transport of solutes have focussed on two large experiments, that give relevant insights into this subject - the long-term pumping and tracer test LPT-2 conducted in 1990-1991 and the study of the flow of saline water during the tunnel excavation.

Methods

Large scale tracer tests are difficult to perform and interpret but are useful to obtain information on large scale connectivity. Test methods and methodology for evaluation need further development

A few deep boreholes for sampling of groundwater and for hydraulic testing are needed also to support the modelling of solute transpor.

CONCLUDING REMARKS

Inter-disciplinary work was performed throughout the investigations to ensure model consistency. To facilitate integration, only four principal investigators with broad responsibilities were involved in the science management. Important definitions, classifications and main issues were defined in the beginning of the site investigation. It is important to have definitions and classification systems defined as good as possible at the outset of a site investigation.

The results and experience from Äspö are partly general in nature and partly sitespecific and they should be relevant for planned site characterization in the Swedish bedrock. If these findings are transferred to other types of bedrock and target depths appropriate modifications of the characterization and modelling programme could be required.

In site characterization for a deep repository, methods should only be used that have been shown to be useful and feasible in practice. Should new methods be considered in the site investigations for the deep repository the Äspö facility will provide excellent conditions for testing prior to application at a real site.

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Session 2a

Characterization methods

A CASE HISTORY OF THE DIFFERENCE FLOW MEASUREMENT AT THE HÄSTHOLMEN SITE IN LOVIISA

Pekka Rouhiainen PRG-Tec Oy, Espoo Finland

Abstract

The difference flow measurement is used to obtain the following results:

- 1. Fresh water head in the borehole with and without pumping from the borehole.
- 2. Flows into or out from the borehole sections with and without pumping from the borehole.
- 3. Fresh water head of the zones or fractures.
- 4. Hydraulic conductivity of the zones or fractures.
- 5 Detailed flow log with 10 cm point intervals.
- 6. Single point resistance log.

The fresh water head measurements were repeated to check the stability in the pressure conditions measured with and without pumping water from the borehole. Flows were also measured with and without pumping water from the borehole. These results can be converted to fresh water head and hydraulic conductivity of fractures. The detailed flow log and single point resistance log are used for exact depth determination of leaky and non leaky fractures.

1 Introduction

The Hästholmen site in Loviisa is one of the four investigation sites in Finland for the final disposal of spent nuclear fuel. Hästholmen is an island, the bedrock is rapakivi granite, groundwater is saline and groundwater level has went down because of the tunnels excavated for low and medium level wastes.

The difference flow method has been used in all the five sites, however, the examples presented here are from the Hästholmen site. The method was developed by PRG-Tec Oy for Posiva Oy, the company which is responsible of the final disposal of spent fuel in Finland.

2 Description of the method

The flowmeter using the difference flow method can be employed to measure groundwater flow into or out from a given borehole section. Measurements can be performed with or without pumping water from the hole. Hydraulic conductivity and hydraulic head in fractures or fractured zones can be deduced from the results if certain assumptions are made.

The new method is a development of the conventional measurement of flow along the borehole. However, it is not the flow along the hole, but the changes of flow with depth that are useful when interpreting the results. Measurement of flow along a hole is problematic especially when the flow is strong because small changes in the flow may be concealed. This problem can be avoided if the changes of flow are measured directly.

With the new flow guide, flow along the hole is directed so that it does not come into contact with the flow sensor. The flow into or out from the borehole in the test section is the only flow that passes through the flow sensor. Instead of inflatable packers, rubber disks are used at both ends of the flow guide. These isolate the borehole section to be measured, see Figure 2.1. The measurements are made essentially in open borehole conditions including that part of the borehole which is under test, Rouhiainen and Pöllänen (1998) and Rouhiainen and Heikkinen (1998)

The interpretation of hydraulic head and hydraulic conductivity implies that the depth sections are measured with two different fresh water heads in the borehole. In fresh water filled boreholes the fresh water head is constant. The groundwater in the Hästholmen site is saline and fresh water head had to be measured. A single difference flow measurement at one depth interval normally takes 12 minutes. This time includes waiting time for temperature stabilisation, a flow measurement by the thermal pulse method, a flow measurement by the thermal dilution method and lifting of the cable to the next depth interval. The thermal dilution method is used to expand the range of measurement to include higher flow rates. The range of flow measurement is 0.1

- 5000 ml/min. Temperature and single point resistance are measured along with the flow rate.

For interpretation of hydraulic head and hydraulic conductivity, a static and cylindrical flow geometry as well as a known radius of influence are assumed.



Figure 2-1. Principle of difference flow measurement

3 Fresh water head in the borehole

The difference flow measurements are carried out with and without pumping water from the borehole. In saline conditions, fresh water head during the measurements have to be determined for interpretation of hydraulic conductivity and head.

Fresh water head in the borehole was measured with a fresh water filled nylon tube. The water level in the tube determines fresh water head in the borehole at the lower end of the tube.

This measurement is normally carried out during the flow measurement. However, a different approach was tested in borehole KR4. The fresh water head measurements were carried out before and after the flow measurements. This has an advantage that automatic logging mode could be exploited in the flow measurements. The flow measurements were carried out unmanned during the nights as well.

The repeated measurement showed that the amount of change of head remained at the acceptable level both with pumping and without pumping, see Figure 3-1. The mean value of the pair was used in the interpretation conductivity and head of fractures.



Figure 3-1 Fresh water head in the borehole before and after flow measurements, reference level Z= 0.89 m, Hästholmen, borehole KR4.

4 Flow and hydraulic conductivity

The measured flows are plotted using a logarithmic scale, see Figure 4-1. The flows are shown in both directions, the left hand side of each diagram represents flow out from the borehole within a test section and the right hand side represents flow into the borehole within a test section. The length of the section was two metres. Flows were measured with and without pumping, see Figure 3-1.

Fresh water head and conductivity of fractures can be calculated from the flows with the assumptions mentioned in Chapter 2. Fresh water head can be calculated if both of the flows at the same depth are not equal to zero, see Figure 3-2. For comparison, fresh water head in the borehole without pumping is also plotted along with the calculated fresh water head of fractures.

Hydraulic conductivity can be calculated if both or either of the flows are not equal to zero. The lower limit of the calculated conductivity depends on the lower limit of the flow range (6 ml/h), the difference between the heads used and on the section length. The points of no flow are plotted on this line of the estimated lower limit of conductivity.

The error bars in Figure 4-2 are obtained assuming that there is always errors in the flow and pressure measurements and that these errors sum up with the worst possible way in the interpretation, Rouhiainen and Pöllänen (1998).



Figure 4-1 Flow rates with and without pumping, length of section 2 m, Hästholmen, borehole KR4.



Figure 4-2 Fresh water head and hydraulic conductivity of fractures, length of section 2 m, Hästholmen, borehole KR4.

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5 Detailed flow and single point resistance logs

A detailed flow logging was performed in the boreholes with 10 cm point intervals. This method provides the depth and thickness of the conductive zones with a depth resolution of 10 cm. To make measurements more quickly, only the thermal dilution method was used for flow determination

The section length chosen was one meter. The width of a flow anomaly of a single fracture is also one meter, respectively. If the distance between leaky fractures is less than one meter the anomalies will be overlapped, see Figure 5-1.

The single point resistance was measured simultaneously with the detailed flow log. For comparison, an ordinary single point resistance result is also plotted, see Figure 5-1. It is hardly possible to detect any of the measured fractures in Figure 5-1 by the ordinary single point resistance method. The single point resistance log of the flow meter is more sensitive because the electrode is installed between the upper rubber disks. The rubber disks obstruct both water and electric charge flow along the borehole.

5 Conclusions

The measurement of fresh water head in the open borehole defines the salinity distribution in the borehole. The repeated measurements made sure the stability of the hydraulic conditions.

The flow measurements were performed in automatic logging mode. An exceptional feature in borehole KR4 was found at depths of 520 - 560 m and 740 - 750 m. The measured flows were approximately equal with and without pumping, see figure 4-1. The angles of the head curves (changes in salinity) hit to these depths, see figure 3-1. A notably negative fresh water head in these fractures could explain the result. Such condition is not impossible because there are tunnels for low and medium level wastes built in the vicinity.

The detailed flow log and single point resistance log are used for exact depth determination of leaky and non leaky fractures. This system makes it possible to find the same fractures for example in borehole TV results. Information of separate fractures can be combined with other data such directional information of them.



Figure 5-1 Detailed flow log with 0.1 m point interval and 1 m section length, single point resistance logs, Hästholmen, borehole KR4.

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ON THE USE OF BOREHOLE RADAR MEASUREMENTS FOR 3D ASSESSMENT OF STRUCTURES IN ROCK VOLUMES

Sven A. Tirén

GEOSIGMA AB, Box 894, S-751 08 Uppsala, Sweden. (sven.tiren@geosigma.se)

Abstract

Construction of a three-dimensional model of an area, for example a site for radioactive waste disposal, requires subsurface extrapolation of surface data and interpolation of subsurface and surface data. Such structural interpretation is based on local information in the perspective of the regional structural setting of the site. This implies that the structural framework of the site has to be inferred from quantitative and qualitative geometrical analysis.

The SKB borehole radar, which can detect structures within a radius of 15 to 25 m around the borehole, is one of the most important sources of geometrical information from boreholes. Directional borehole radar measurements produce information on the angle (α) at which a feature intersects the borehole and the location (azimuth) relative to the borehole. Although the azimuthal information is important for the subsequent interpretation, the critical parameter that determines whether the feature is detected by the radar appears to be the α -angle. In this paper, the performance of the radar tool concerning α -angles is studied. The reason for undertaking the study was that predicted low angle intersections between boreholes and structures were not identified. This suggests that the relationship between the sampled population and the target population needs to be investigated. The analysed data sets comprise 307 reflectors from the Romuvaara site in Finland and 307 reflectors from the cored boreholes in the Hard Rock Laboratory (HRL) at Äspö, southeastern coast of Sweden.

In the Äspö bedrock, the shape of the frequency histogram displaying the α -angles is very consistent throughout the area. A brief comparison of amplitudes and reflectivity shows that the shape of the frequency histogram is tool-dependent rather than depending on the physical properties of the zones. The potential of the borehole radar to detect structures intersecting the borehole at very high angles (75° to 90°) is low due to the transmitter-receiver configuration of the tool. In the Äspö radar data, the range of the borehole radar appears to be narrower than expected, with very few radar reflectors at angles above c. 60°. This could indicate that the measured radar velocity is too low (c. 20%).

This implies that target structures investigated by a single borehole should be intersected at an angle of about 30°. For further drilling it is noteworthy that an orthogonal borehole would not add new information to the first hole concerning the sectors with poor radar detection. Full coverage of structures within an area demands a drilling program that considers the bias in the borehole radar sampling. An accurate determination of the radar wave velocity is essential for correct orientation of radar reflectors.

1. Introduction

The Swedish Nuclear Power Inspectorate (SKI) has conducted an integrated performance assessment study, the SKI SITE-94 project (SKI, 1996), using surface-based Äspö data collected by the Swedish Nuclear Fuel and Waste Management Co. (SKB) in their research and development of storage of nuclear waste. The SITE-94 project is followed by an investigation including also subsurface data (Äspö Hard Rock Laboratory, HRL). An important task of the SKI investigations is to study the uncertainties in the methods used for acquisition, evaluation and modelling of data (cf. Tirén et al., 1996).

In structural modelling access to oriented data is essential. Geometrical data describing fractures and fracture patterns on exposed rock (outcrops and tunnels) are compiled by detailed mapping. Remote sensing, e.g. structural interpretation of topographical data and airborne geophysics gives the structural pattern on the surface on local to regional scale. This information can be complemented with surface geophysics, such as reflection seismics. The borehole radar, used by SKB for site characterisation, provides oriented data on a scale in between surface measurements and mapping of exposed rock. The joint use of multi-scale data contributes to the confidence in each individual data set. Examples of such data are detailed geophysical measurements, detailed geological field data, borehole logs and core logs.

In the SKI SITE-94 work, the borehole radar has been the principal source of oriented data (Tirén et al., 1996). Analysis of the data shows that there is an unexpected low number of reflectors intersecting the borehole at low angles. This suggests the presence of undocumented restraints on the angular detection capabilities of the radar tool. Consequently, the relationship between the target and the sampled populations needs to be investigated.

This paper discusses the performance of the radar tool, with emphasis on the angle of intersection between the borehole and the reflector (α -angle), exemplified with data from two areas, Romuvaara in Finland and Äspö in Sweden. The present paper is a short version of a forthcoming SKI-report (Tirén et al, in preparation).

2. Radar sample

The quality of the sample achieved by borehole radar measurements is related to the ability of the borehole radar to detect objects (e.g. depending on their physical contrast between features and the bedrock) and the sampled volume. Frequency dependent electrical properties of the rock mass govern the propagation of the radar waves and consequently the sampled volume. The potential of the borehole radar to detect structures intersecting the borehole at a very high angle (75° to 90°) is low due to the transmitter-receiver configuration in the radar instrument (Olsson et al., 1990).

The orientation of a radar reflector is first determined relative to the borehole (α -angle and azimuth) and subsequently recalculated to an absolute orientation in terms of strike and dip. The recalculation is based on the borehole deviation measurements. Hence, the

location of a discrete reflector is given by its intersection with the borehole or the intersection with the extension of the borehole. Location of a reflector parallel to the borehole is given by its relative azimuth to the borehole and its distance to the borehole, calculated as a function of the velocity of the propagation of the radar wave. An erroneous propagation velocity affects the α -angle (but not the azimuth), and thereby the absolute orientation of the feature. Consequently, the study of the borehole radar's ability to detect and orient a feature can be restricted to a study of the α -angle.

3. Romuvaara site

The Romuvaara site in eastern Finland (cf. Saksa, 1992) is composed of Archean gneisses. Borehole radar surveys have been performed in eight steeply to vertical plunging boreholes, five of them plunging steeply eastwards. A total of 307 reflectors were found in the Romuvaara boreholes, Figure 3-1. The total surveyed length is 4080.5 m.

The poles of radar reflectors, in Figure 3-1, cluster along a small circle with an axis plunging steeply eastwards and having a radius of c. 60°. Vertical radar reflectors are scarce. When plotting only radar reflectors from the five steeply south-eastwards plunging boreholes, the circular structure on the stereogram is more accentuated. The pattern, exhibited by the radar reflectors recorded in the three boreholes with the most divergent orientations (steeply plunging N, E and S), appears quite deviating. The dominant orientations of fractures within the Romuvaara site (Saksa et al., 1992) do not coincide with the orientations of the radar reflectors, with only few exceptions.



Figure 3-1 Orientations of borehole radar reflectors in the Romuvaara site, eastern Finland: a) All reflectors (307), poles of dominant fracture orientations (white dots) and orientation of boreholes (grey dots), b) Orientations of radar reflectors (200) detected in steeply eastwards plunging boreholes, and c) Orientations of radar reflectors (107) detected in three boreholes steeply plunging northwards, eastwards and southwards, respectively. Equal area, lower hemisphere projection. Contouring 1%, 2% and 3%.

The α -angle frequency histogram from the Romuvaara site displays an irregular pattern. The distribution appears to be bimodal with maximum at c. 30° and c. 45°, respectively, Figure 4-2.
4. Äspö HRL

4.1. Borehole configuration and radar data

The HRL is a 500 m deep construction excavated in approximately 1.8 Ga old grantoids. The number of oriented radar reflectors is 307, the total length of the surveyed borehole length is 2815.5 m and the number of boreholes is 24. The configuration of holes drilled from the Äspö HRL, surveyed by the borehole radar, are oriented in two sectors. The majority of the boreholes (20) are oriented within the sector NE-SW to SE-NW (total borehole length 2974 m, 2433 m surveyed by borehole radar). The remaining holes (4) are in the sector SSE-NNW to N-S (total borehole length 630 m, 383 m surveyed by borehole radar).

Vertical radar reflectors striking WNW-ESE are abundant, Figure 4-1. Furthermore, several are NNE-SSW striking reflectors dipping steeply to vertical toward SE and NW. A system of greatly to moderately dipping reflectors striking approximately NE-SW is indicated. Notable is the subordinate occurrence of vertical radar reflectors striking NNW-SSE and WSW-ENE, structures considered to be important during the initial surface-based investigations.



Figure 4-1 Orientations of borehole radar reflectors (307) in the Äspö HRL boreholes (left) and borehole radar reflectors (56) in surface-based Äspö boreholes. Equal area, lower hemisphere projection. Contouring 1%, 2% and 3%. Grey dots are cored boreholes (24 HRL and 3 surface-based boreholes).

The pattern of radar reflectors recorded in three surface boreholes is not fully consistent with radar pattern in the HRL boreholes. Significant is the difference in the steeply dipping NNW-SSE and ENE-WSW striking reflectors.

4.2. Detailed analyses of the α -angles

The frequency of α -angles in the HRL varies, Figure 4-2. A maximum occurs in the interval of 30° to 34° and there is a marked drop for α -angles smaller than 25° and a regular decrease from 35° to 60°. The number of α -angles greater than 60° and less than 15° is relatively few (less than 2% and 6%, respectively). The distribution of α -angles in surface-based Äspö boreholes (337: 281 semi-oriented reflectors in 9 boreholes and 56

oriented reflectors in 3 boreholes) show a similar pattern as that for the HRL borehole radar reflectors (cf. Tirén et al., 1996).



4.2.1. Orientation of reflectors vs. α -angles

The configuration of HRL boreholes is dominated in number by boreholes oriented approximately E-W. However, boreholes plunging south-westwards have a longer total borehole length. As the sampling is not uniform in all directions, the direction of some of the orientation of radar reflectors may be enhanced. By sorting reflectors according to their α -angle, this can be checked.

For small α -angles (0° to 9°) the reflectors have an approximately E-W strike with various dips. A transition occurs for greater α -angles (10° to 19°) where no dominant strike exists. Furthermore, the fraction of steep reflectors increases. For α -angles between 20° and 40° WNW-ESE/vertical fractures are dominant. An orthogonal steeply dipping fracture system appears for α -angles in the interval 40° to 49°, striking WNW-ESE and NNE-SSW. At still greater α -angles (greater than 50°) the pattern of radar reflectors becomes indistinct, while steeply dipping reflectors are indicated. There are only three reflectors with α -angles greater than 60°.

4.2.2. Magnitude of reflectors vs. α - angles

The magnitude of a radar reflector can be assumed to vary with the physical character of the reflector and the angle of incidence. All recorded borehole radar reflectors are classified according to the scale: Strong (36), Medium (81), Weak (116), and Uncertain (74).

The frequency histograms of the Weak and Uncertain reflectors look very much like the frequency distribution of all reflectors, cf. Figure 4-2. The Strong and Medium reflectors, on the other hand, both show significant peaks for narrow direction intervals, 25° to 29° and 30° to 34° , respectively.

There appears to be a relation between the magnitude of reflectors and its orientation:

• Strong reflectors have a dominating dip of 30° to 60° north-eastwards.

- Medium reflectors consist of two steeply dipping sets with strikes in WNW-ESE and NNE-SSW and a set of structures dipping 30° to 60° southeastwards.
- Weak reflectors are WNW-ESE striking, steeply dipping
- Uncertain reflectors strike NE-SW, steeply dipping.

4.2.3. <u>Comparison with core log data</u>

Core logs for some boreholes surveyed by borehole radar have been available, and α -angles of borehole radar reflectors were compared with α -angles of natural fractures (fractures parting the core), sealed fractures, lithological contacts and veins. Natural fractures and sealed fractures both have maximum for fracture-borehole intersection angles of 45° to 49° and both types of fractures show frequency distribution histograms indicating normal distributions. Unfortunately, oriented data are not available.

The reasons for a maximum at c. 45° have to be studied further as the borehole radar reflectors have a maximum at c. 30° . A simple calculation only considering the dominant WNW-ESE/subvertical fracture set in the HRL and orientations and lengths of boreholes, shows that fractures intersecting the boreholes at c. 45° will dominate.

4.2.4. <u>Comparison with fracture mapping in the HRL</u>

There are two sets of data from the tunnel work, fracture logs and fracture zone logs. A subset of all mapped fractures (about 10% or approximately 1000 fractures) are denoted wet, Figure 4-3. The wet fractures strike WNW-ENE and have a vertical dip. Fracture zones are mapped at 115 locations in the HRL. These zone strike around NE-SW with dominating dips towards the southeast. It is noteworthy that fracture zones parallel to the dominating water-bearing fracture set are scarce, Figure 4-3 (see also Figures in Tirén and Voss, this volume). Fracture zones in the HRL have orientations similar to the orientations of fractures that outlining the form of outcrops, Figure 4-3.



Figure 4-3 a) Wet fractures (998) and b) fracture zones (115) mapped in the HRL main tunnel. c) Fractures outlining the morphology of outcrops (702). Contouring 1%, 2% and 3%.

5. Discussion of results

The most frequently sampled structures are those intersecting the borehole or its extension at an angle of c. 30° while structures intersecting the borehole at angles within intervals of 0° to c.15° and c. 60° to 90° are relatively few. The shape of the distribution curve for α -angles obtained in the interval from 0° to c. 60° is empirical and diverges, from what could be expected from theoretical considerations (cf. Falk, 1992).

The theoretical explanation for the low number of detected structures intersecting at high angles, 75° to 90° is the antenna configuration, i.e. a tool dependent restraint. The Äspö sample, however, lacks reflectors with an α -angles larger than c. 60°. A plausible explanation for this is that the measured propagation velocity of the radar wave is too low. An adjustment of c. 20%, which represents an increase from 100 to 123 m/µs will revise the upper boundary from 60° to 75°. However, such an adjustment needs a recalculation of the orientation of all reflectors.

The regular increase in the number of detected structures from α -angles from 60° to c. 30° may reflect the change in reflection coefficient. It increases as the angle of incidence increases and should have a maximum at 90° (cf. Falk, 1992), i.e. for reflectors parallel to the borehole (α -angle equal to zero). The reason for the relatively rapid decrease of detected reflectors with α -angles smaller than 30° is speculative. One possibility could be the contrast in the physical properties of the structure versus the host rock (dielectric constant, resistivity, reflection and refraction of radar waves) which will affect the reflectivity of the structure.

Core log data indicate a $45^{\circ} \alpha$ -angle maximum for discrete structures, which differs from the 30° maximum of the borehole radar reflectors. There is no trace of a 45° maximum in the radar data.

The sample of oriented structures obtained with the borehole radar in the Romuvaara site appears to be related to the orientation of the boreholes. This is further emphasised by the fact that there are several sets of steeply dipping and sub-horizontal fractures that have not been detected by the borehole radar (cf. Saksa et al., 1992). The α -angles of the vertical structures are all less than 30°, which implies that the ability of the borehole radar to detect the structures is reduced. A similar explanation can be given for the gently inclined to sub-horizontal fracture sets, but here the α -angle is greater than c. 60°. This implies that the borehole configuration in the Romuvaara site is not favourable to detect the dominant fracture sets in the area. Instead, the borehole radar surveys enhance structures that have a favourable orientation to be detected by the borehole radar. This results in a biased sample, but the structures causing the reflections still have to be explained. There is also a relatively high number of reflectors with low α -angles compared to the Äspö sample. In spite of this, the frequency distribution expressed in the Äspö sample is recognisable in the Romuvaara sample.

On Äspö the surveys performed from the surface have detected features with significantly different orientations compared to the features located in the HRL holes, Figure 4-1. This difference is probably due to an effect of sampling bias, since most boreholes on the surface are almost perpendicular to the holes drilled in the HRL.

Further studies of the α -angles of radar reflectors in additional areas will increase knowledge of what eventually could be site specific characteristics and what could be a general bias in the structural sampling conducted with the borehole radar. In Sweden all borehole radar surveys performed by SKB in order to characterise areas prior to the investigation of the Äspö HRL, i.e. before c. 1990, have employed dipole antennas since the directional antenna was first introduced during the "pre-investigation" study of the Äspö HRL study. This implies that only relative orientations of reflectors were obtained in the earlier studies, that is the α -angles, which limits the use of studies of Swedish areas. In Finland, on the other hand, there are still three more areas investigated with the directional borehole radar.

6. Conclusions

The borehole radar is an extremely vital tool for the structural understanding of fractured crystalline rock. In many places, there are no significant characteristics of fracture zones in different directions due to repeated deformation along, and partial reactivation of, faults. In such cases the reflectors detected by the radar, primarily due to their extension or size, will be the main tool to depict the structural framework in the bedrock. The data presented here show that the radar excels at fracture detection within a certain α -angle interval. Outside this interval, the performance of the radar deteriorates quickly. This relationship appears to be tool dependent. The effect of sampling (cf. the Terzaghi correction for scanline sampling) may contribute to decrease the sample of structures intersecting a borehole at a small α -angles. However, it could not explain why such structures are badly detected in the Äspö bedrock. This can, if not considered, effect how well a model will depict the structural framework in the bedrock.

Apparently the ability of the borehole radar has a maximum when intersecting structures at an angle of c. 30° and it diminishes rapidly for lower intersection angles and more slowly for higher intersection angles. At high intersection angles, the ability to detect structures is lowest. This geometrical relationship has to be considered when planning borehole radar surveys and especially when the target will be investigated from several holes drilled in different directions. The target could be a specific object as a fracture zone, but it could also be a rock volume. An orthogonal borehole configuration does not optimise the potential of the borehole radar, as there will be orientations of structures poorly sampled by all boreholes.

Due to uncertainties in the sampling, borehole radar data for statistical models should be used conscientiously.

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VSP IN CRYSTALLINE ROCKS - FROM DOWNHOLE VELOCITY PROFILING TO 3-D FRACTURE MAPPING

Calin Cosma, Pekka Heikkinen, Jukka Keskinen and Nicoleta Enescu Vibrometric Oy, Helsinki, Finland

Abstract

VSP surveys have been carried out at several potential nuclear waste disposal sites in Finland since the mid 80's. To date, more than 200 three-component profiles have been measured. The main purpose of the surveys was to detect fracture zones in the crystalline bedrock and to determine their position.

Most seismic events could be linked to zones of increased fracturing observed in the borehole logs. The more pronounced seismic reflectors could be correlated with hydrogeologically significant zones, which have been the main targets in the investigations.

Processing and interpretation methods have been developed specifically for VSP surveys in crystalline rocks:

- Weak reflections from thin fracture zones are enhanced by multi-channel filtering techniques based on the Radon transform.
- The position and orientation of the fracture zones are determined by polarisation analysis and by combining data from several shot points.
- The compilation of the results from several boreholes gives a comprehensive image of the fracture zones at the scale of the whole site.

The discussion of the methodology is based on examples from the Olkiluoto site, in SW Finland.

1 Introduction

Vertical Seismic Profiling has routinely been used as a means of improving the interpretation of the surface reflection surveys in sedimentary basins. Since the late 80's VSP also became a favoured methodology for deep seismic imaging, especially in crystalline rocks. The basic reasons for this development are as follows:

- With VSP, the source and the detectors can be placed within the bedrock itself, the loss of resolution due to near-surface signal absorption being largely avoided.
- 3-component detectors allow the polarisation of the signals to be used as an indication of the orientation of the reflectors. Even if 3-component receivers were used with surface profiling, most of the polarisation information would be lost due to near surface refraction, which causes all signals to arrive at the detectors on nearly vertical paths.
- The arrays of receivers placed in vertical or steeply inclined boreholes provide a favourable geometry for mapping, in depth, steeply dipping fractures.
- VSP is, generally, a more economical solution than a 3D surface seismic survey.

The capabilities of the VSP imaging method include:

- obtaining accurate velocity estimates in depth,
- determining rock mass anisotropy,
- mapping fracture zones and lithological contacts in 3-D.

Several authors reported good results with the first two topics above (Leary at al., 1989), (Rector, 1989), (Söllner et al., 1992), (Miao et al., 1995). The third topic is complex and includes the first two, among others. So far, most of the references to this topic relate to Radioactive Waste Management, e.g. (Cosma and Heikkinen, 1995).

The Site Investigation Programme for the Final Disposal of Spent Nuclear Fuel in Finland started in 1983 and the preliminary site investigations begun in 1987. Since then, more than 200 three-component VSP-surveys were carried out at several sites, often to depths approaching or exceeding 1000 m. The main objective of these surveys was to detect fracture zones in the crystalline bedrock and determine their position and orientation.

New processing and interpretation techniques were needed to turn VSP into a tool for mapping fracture zones. The reflections from fractures in crystalline rock are generally less pronounced than those from the boundaries of sedimentary formations, while scattering is stronger. Moreover, unlike reflections from sedimentary formations, in crystalline rocks the reflecting boundaries can have any orientation and 2-D analyses are not applicable.

Currently, the rock models of the sites investigated and in particular the deeper sections rely strongly on the results of the VSP surveys.

2 Methodology

2.1 Data acquisition

The deep boreholes drilled during the investigations in crystalline rocks are often slim, even when the depth exceeds 1000 m. The combined requirements of small size, wide frequency band, 3-D directional sensitivity, high data production rate and relatively low cost were difficult to meet with existing seismic exploration equipment.

A multi-level 3-component receiver chain, with an outside diameter of 43 mm, was designed and built for surveys in slim boreholes. The optimum number of levels allowing manual handling is 8, but it can be increased to 16 for higher data production. Each module is equipped with geophones or accelerometers and preamplifiers. The modules clamp to the hole by side arms activated by DC motors (*Figure 2-1*).

At the kilometre scale, the P-wave frequencies recorded can go up to 500 Hz. The corresponding S-wave maximum frequency is roughly 300 Hz. In both cases the minimum wavelength is approximately 12 m. Therefore, the distance between the levels in the receiver chain is 5 m, i.e. slightly less than the half of the minimum wavelength. This allows the detection of rock features with thickness of 1 metre, or even less. For surveys at smaller scales interlaced records are taken, e.g. at 2.5 m, to avoid spatial aliasing due to the possibly higher frequency content of the signals.



Figure 2-1. The multi-level borehole seismic receiver chain for deep VSP surveys. It contains eight 3component receiver modules clamped to the borehole by a side arm mechanism. The clamping arm is moved by an electric motor.

In areas with thin overburden, a handy way to produce VSP signals is by placing small dynamite charges (35 - 70 g) in shallow holes drilled into the bedrock. Typically, a group of three holes are drilled at each shot point and the shooting is switched from one to another in case of collapse. This arrangement becomes uneconomical in areas covered by thick overburden where deeper holes are needed to reach the bedrock. In these situations engineered sources, e.g. borehole guns and hammers, are preferred, as the risk of

collapse is much smaller than with explosives and one shot hole is normally sufficient for measuring a whole VSP profile.

With VSP, the angular coverage is more complete than with surface reflection profiling. Therefore, VSP will be more successful in determining the geometry of the rock features, especially of the steep ones. Conversely the positional coverage is less complete and only certain portions of these features can be imaged by any single VSP survey. To resolve this, VSP surveys are conducted in several boreholes, with each subsequent survey partly overlapping the previous ones but also contributing with new information, from other regions of the site, until a complete and iteratively validated model is obtained.

At the initial site description stage, the investigation area is of the order of 10 km^2 . A fairly complete coverage was achieved at the Olkiluoto site, in SW Finland, with nine boreholes with depths ranging from 300 to 1000 metres. The average distance between the boreholes was 500 metres. A spread of six to nine shot points was set around each borehole, with offsets varying from 100 to 500 metres.

2.2 Velocity Models and Anisotropy

VSP is used in sedimentary formations for determining the 'interval velocities', which are required for depth-migrating surface reflection data. A similar approach can be used in crystalline rocks, if the shots are placed in the bedrock, as recommended in the previous section. In this case, it can assumed that significant velocity variations occur only in the near-surface weathered zone, hence the velocity field can be considered one-dimensional (nonetheless, a ray tracing inversion approach is needed for determining the velocity-depth function for shots with significant horizontal offsets). *Figure 2-2* depicts the fracture density log, the sonic log and the VSP interval velocity measured in the same



borehole (KR4). One can see that the acoustic log is indicative verv of the fracture density, while the thin fracture zones are not observed in the velocity function computed from the VSP data (the dashed line in Figure 2-2). The lack of significant velocity а contrast in depth makes the relevance of the interval velocity procedure questionable in crystalline rocks.

Figure 2-2. The fracture density log (bottom picture), the sonic log and the VSP interval velocity (top picture) measured in borehole KR4 (Olkiluoto).

A velocity model becomes essential when thick overburden prevents the shots from being placed in the bedrock. As the overburden-bedrock interface is not necessarily horizontal, a one-dimensional velocity model may not be always suitable and more intricate approaches must be devised. *Figure 2-3* presents a case where the determination of the velocity function has been derived by 3-D tomographic inversion using ray tracing. The survey layout consisted of 3 deep boreholes, with two shot points for each borehole. Ray tracing was applied. The tomographic velocity distribution is shown in the plane of the maximum dip of the overburden-bedrock contact. Although the 3-D VSP tomographic inversion shown in *Figure 2-3* provides no direct information on the structure of the bedrock, it determines the reliability of the geometrical model obtained as a final result.



Figure 2-3. 3-D velocity model, shown in the plane of the maximum dip of the overburden-bedrock contact.

As shown in *Figures 2-2* and 2-3, velocity variations within the rock mass due to local changes of the rock texture are generally small. However, anisotropy is quite common and is often related to trends in the orientations of the fractures.

As an example, *Figure 2-4a* shows the P-wave velocities determined from first arrivals as a function of the receiver depth, for the six profiles measured in borehole KR6 at Olkiluoto. It can be seen that the velocities vary considerably and it was not possible to construct an isotropic velocity model to account for the anomalous velocity-depth functions in all six profiles. The rockmass was therefore modelled as a transversely isotropic medium (Thomsen, 1986), in which the minimum velocity is normal to the dominant fracturing. With this approach, the velocity function can be described by the values of the maximum and minimum velocities and by the direction of the axis of minimum velocity.

Figure 2-4b presents the velocity-depth function for profile L22, which displays the most anomalous variation in Figure 2-4a. The velocity function corresponding to the transverse isotropy model is shown for comparison. The parameters of the model have the following values: minimum velocity 5.1 km/s, maximum velocity 6.1 km/s, and direction of the minimum velocity dipping approximately 20° to N-NE. It is apparent that the velocity variation is overwhelmingly due to anisotropy. After subtracting the anisotropic component the velocity variation was reduced to less than +/- 100 m/s.



Figure 2-4a (left). P-wave velocities determined from first arrivals as a function of the receiver depth, for the six profiles measured in borehole KR6 at Olkiluoto.

Figure 2-4a (right). The velocity-depth function for profile L22.

2.3 Modelling the 3-D Fracture Geometry

The preliminary processing consists of a series of fairly standard procedures aimed at emphasising the reflected field. The typical steps of the preliminary processing stage are the following:

- indexing the traces and synchronising the traces with the survey coordinates,
- picking arrival times,
- rotating the horizontal components to the radial (R) and transversal (T) directions,
- band-pass filtering,
- removing direct P-waves, S-waves and tube-waves by median filter,
- deconvolution,
- amplitude compensation using the same AGC-operator for all three components.

A thorough checking of the data is performed during this stage and, where needed, other means of signal conditioning are also applied, e.g. static corrections based on heterogeneous and/or anisotropic velocity models, as discussed in the previous section.

The stronger reflections can generally be pinpointed in the pre-processed data. A common attempt to make them more visible is exemplified in *Figure 2-5*. The procedure consists of shifting the traces along the time axis by an additional interval equal to their respective travel time and stacking them. In zero-offset sections, horizontal reflectors appear as synchronous and are emphasised by stacking (*Figure 2-5b*). The technique is hardly of any use in crystalline rocks, where horizontality has no particular meaning and large shot offsets are the rule, rather than the exception. *Figure 3-1b* shows a corridor stack for data acquired in a crystalline rock environment and this illustrates that this is a rather poor means of enhancing reflectors.



In crystalline rocks, reflectors are generally masked by scattering, surface multiples, converted waves, tube-waves and stronger reflections. Multi-channel filters based on a version of the Radon transform - the Image Point transform - are used for enhancing weak reflections and for separating the interfering events (Cosma and Heikkinen, 1995). The effect of the technique is exemplified in *Figure 3-1c*.

Figure 2-5. Zero-offset and stacked sections.

The filtering capabilities of the Image Point transform result from the fact that reflectors with different orientations are imaged in different regions of the transform space and that the actual propagation velocity is used instead of the apparent velocity, as the case is e.g. with the τ -p transform. Enhancing reflectors with different orientations is reduced to simple editing of the transform space.

3 3-D Modelling

A notable characteristic of the Image Point approach is that polarisation filters applied in Image Point space avoid the problems appearing in the time-depth representation caused by noise and interference among coherent events with different origins. By using the polarisation of the signal in the Image Point space, it is possible to enhance reflections arriving from specific azimuths and thus estimate the dip direction of the corresponding reflecting interfaces.

The travel time function associated with a planar reflector gives a relation between the dip and the dip direction and, with the dip direction already estimated independently by polarisation, the dip can be computed. The travel time function also determines the

distance from the reflector to the borehole. Therefore, all the three parameters needed to completely determine the position and orientation of a planar reflector are resolved.

Figure 3-1 shows the pre-processed section and the same section after polarisation filtering, from the zero-offset shot point of borehole KR8. The reflectors dipping to South are enhanced. Polarisation filters applied in the Image Point space help in determining the orientations of the reflectors and also enhance the reflected signals, making the determination of their traveltime functions easier.



Figure 3-1. Pre-processed section and the same section after polarisation filtering, from the zero-offset shot point of borehole KR8. The middle section represents a corridor stack.

The orientation estimated by polarisation analysis is usually no better than +/- 10° but the results is very robust. The estimate can be significantly improved by combining the results from several shot points and in some cases, by using the converted (P-to-SV) reflections. In the far-offset sections conversions have a different variation with dip and dip direction than the P-wave reflections. Due to the sparseness of the coverage offered by small number of shot-points, this procedure is carried out by statistical analysis, rather than by linear integration. This makes it relatively unstable, meaning that small errors in the input may produce large changes in the model. After determining the average position and orientation of a reflector, those regions actually mapped can be computed.

4 Application of 3-D Fracture Mapping

Most of the reflectors detected by VSP in crystalline rock can be interpreted as fracture zones, appearing in the borehole logs to be from 2-3 m to 30-50 m thick, with a typical fracture density of 10 pcs/m. The velocity change resulting from the presence of such fracture zones is of the order of 10 %, or more. Within a signal frequency range of 200-600 Hz, it is possible to image fracture zones less than 2 m thick. Fracture zones more than 30 m apart, i.e. 2-3 wavelengths, can be positively resolved as separate reflectors.

These conclusions are confirmed by the results from Olkiluoto. The three strong reflections (A, B and C) from *Figure 4-1b* can be correlated with fracture zones seen at the depths 85-90 m, 320-380 m and 760-800 m in the P-wave sonic and fracture logs in *Figure 2-2*. The fracture zones at the depths 520 m and 650 m are better imaged from other shot points. A closer examination of the section in *Figure 4-1* reveals that the event B consists of two reflections, corresponding in the logs in Figure 2-2 to 3-5 m thick fracture zones, at 320 m and 360 m depth.

The reflector C also consists of two branches, representing fracture zones at the depths of 760 and 790 m. The event D does not intersect the borehole but can be correlated with a fracture zone found in the nearby hole KR2, as seen in *Figure 4-1a*.



Figure 4-1a (left). The major fracture zones determined from VSP from boreholes KR4, KR2 and KR8 at Olkiluoto. The fracture zones are marked with A-D.

Figure 4-1b (right). The polarisation-filtered section from shot point L25, borehole KR4. Reflections dipping to the South are enhanced. The strongest reflections (A-D) come from the fracture zones marked in Figure 4-1a.

When the reflector position estimates based on polarisation analysis are improved by combining the results from several shot points, the spread of the dips and dip directions is, usually, a few degrees. As the reflections from different shot points map different areas of the reflecting boundaries, the consistency of the reflector attitudes indicate that the fracture zones are quite planar at least over an area a few hundreds of metres.

Once the geometry of the reflectors has been established, determined as best fitting planes, the areas where the reflections actually occur for different shot points can be computed. Figure 4-1a displays the major fracture zones interpreted from the VSP

surveys performed in boreholes KR4, KR2 and KR8 in Olkiluoto (Cosma et al., 1996). The areas actually mapped by VSP data are shown as small rectangles and the average position of the reflecting planes as grey shaded planes. As seen in Figure 4-1a, most of the reflecting boundaries can be correlated from one borehole to another. The major fracture zones at the Olkiluoto site seem to form a system of zones dipping gently (10-30 degrees) to south.

This observation is also confirmed by hydraulic studies (Paulamäki et al., 1996). The upper boundary of the saline groundwater and the hydraulic flow patterns in the holes were shown to be controlled by the fracture zones. The flow studies also indicate that the fracture zones observed in the two adjacent boreholes (KR4 and KR2) are connected as indicated by the VSP results.

5 Conclusions

The multi-offset three-component VSP can be successfully used in determining the 3D positions of thin fracture zones in crystalline rock, as shown by the results of the VSP measurements at the potential radioactive waste disposal sites in Finland. VSP also images the zones accurately at depths difficult to reach by other methods. The rock fracture zones interpreted from VSP surveys in several boreholes can be combined into a comprehensive site model.

Compared with surface seismic methods, higher frequencies can be used with VSP, which leads to higher resolution. This is due to the fact that both the sources and the receivers can be directly placed in the hard rock.

Due to the relatively high signal frequency, most of the VSP reflectors in crystalline rock can be correlated with fracture zones, with fractures as narrow as 1-2 m being detected and zones separated by 20-30 metres can also be resolved as individual reflectors, within an investigation range of 1-2 km.

The standard VSP processing and interpretation routines are not sufficient for mapping fracture zones in crystalline rock. A more efficient technique is the Image Point transform, which, used in conjunction with polarisation analysis, gives the possibility to enhance weak reflections from thin fracture zones and, simultaneously, to determine their 3D orientation, thus extending the imaging range of the VSP method from the vicinity of the borehole to the site scale.

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REFLECTION SEISMIC METHODS APPLIED TO LOCATING FRACTURE ZONES IN CRYSTALLINE ROCK

Christopher Juhlin

Uppsala University, Dept. of Earth Sciences, Villavägen 16, 75236 Uppsala, Sweden

Abstract

The reflection seismic method is a potentially powerful tool for identifying and localising fracture zones in crystalline rock if used properly. Borehole sonic logs across fracture zones show that they have reduced P-wave velocities compared to the surrounding in-tact rock. Diagnostically important S-wave velocity log information across the fracture zones is generally lacking. Generation of synthetic reflection seismic data and subsequent processing of these data show that structures dipping up towards 70° degrees from horizontal can be reliably imaged using surface seismic methods. Two real case studies where seismic reflection methods have been used to image fracture zones in crystalline rock are presented.

Two examples using reflection seismics are presented. The first is from the 5354 m deep SG-4 borehole in the Middle Urals, Russia where strong seismic reflectors dipping from 25° to 50° are observed on surface seismic reflection data crossing over the borehole. On vertical seismic profile (VSP) data acquired in the borehole, the observed P-wave reflectivity is weak from these zones, however, strong converted P to S waves are observed. This can be explained by the source of the reflectors being fracture zones with a high P wave to S wave velocity ratio compared to the surrounding rock resulting in a high dependence on the angle of incidence for the reflection coefficient. A high P wave to S wave velocity ratio (high Poisson's ratio) is to be expected in fluid filled fractured rock.

The second case is from Ävrö, SE Sweden, where two 1 km long crossing high resolution seismic reflection lines were acquired in October 1996. An E-W line was shot with 5 m geophone and shotpoint spacing and a N-S one with 10 m geophone and shotpoint spacing. An explosive source with a charge size of 100 grams was used along both lines. The data clearly image three major dipping reflectors in the upper 200 ms (600 m). The dipping ones (to the South, East and Northwest) intersect or project to the surface at or close to where surface mapped fracture zones exist. The South dipping reflector correlates with the top of a heavily fractured interval observed in a borehole (KAV01) at about 400 m. 3D effects are clearly apparent in the data and only where the profiles cross can the true orientation of the reflecting events be determined. To properly orient and locate all events observed on the lines requires acquisition of 3D data.

1 Introduction

Reflection seismics have served as a useful tool for imaging and mapping of fracture zones in crystalline rock along 2D lines in nuclear waste disposal studies. (Carswell and Moon 1989; Juhlin 1995; Mair and Green 1981). This also applies to mineral exploration where the targets have been the general structural setting of the ore deposits or the ores themselves (Juhlin et al., 1991; Milkereit et al., 1996; Milkereit et al., 1994; Milkereit et al., 1992; Spencer et al., 1993). Although the primary targets on many of these lines can be approximated as 2D structures it has been evident that there exists numerous out of the plane reflections in the acquired data. This is to be expected in crystalline rock which has been subjected to several phases of deformation and/or metamorphism. In addition, strong P- to S-wave conversions may be expected from fracture zones if they contain significant amounts of fluids. These converted S-waves and the variation of amplitude with angle of incidence for the P-wave reflection coefficient can cause further problems in processing and interpreting seismic reflection data. However, the potential for better characterising the reflectors, and hence the fracture zones, is also possible if both P-wave and S-wave data can be acquired, processed and interpreted properly.

A major concern in the localisation of a nuclear waste site is the presence of hydraulically sub-horizontal fracture zones since these may have a major impact on water circulation patterns once waste has been deployed underground. These subhorizontal to gently dipping fracture zones are difficult to detect using geological mapping methods since they generally do not intersect the surface in the area being mapped. In addition, drilling and hydraulic testing often give data which are difficult to interpret resulting in that borehole to borehole correlations may be poor. Reflection seismics provides a tool for integrating surface studies with borehole results in locating sub-horizontal to gently dipping fracture zones, some which may be hydraulically conductive. Reflection seismics can also constrain the geometry at depth of more steeply dipping known fracture zones which intersect the surface. Since there are numerous factors to consider in choosing a nuclear waste disposal site it is important that the seismic image obtained is as accurate as possible. The presence of subhorizontal events on a seismic line need to be confirmed as truly being sub-horizontal by shooting either several cross lines or, preferably, by acquiring 3D data.

This paper briefly reviews the seismic reflection method, discusses the need for 3D data, and shows how the amplitude of P- and S-waves may vary with angle of incidence. Two examples of real data are presented, one where P- to S- wave conversions are shown to be important and the other where 3D effects are clearly evident in 2D data.

2 Seismic reflection method

Seismic data are generally acquired by exciting a source (explosive, vibrator, etc.) on the surface or in a borehole and recording the waves emanating from this source on an array of receivers (geophones, hydrophones, etc.). Ideally, numerous sources are excited and the acquired data are processed in such a manner so that a subsurface image is obtained that can be interpreted. The method has been, and is, applied with great success in the petroleum industry on sedimentary rock based on the assumptions that interfaces are sub-horizontal and that only acoustic waves are propagating (no shear waves). In crystalline rock these assumptions are often not valid since some of the strongest variations in rock properties may be laterally and shear waves are often generated at interfaces. Even simple models may generate complex seismograms (Figure 2-1). Traditional processing (CDP sort, NMO, stack) of such data will give an image which is incorrect. However, if more advanced processing is applied (pre-stack migration and stack) then an image which resembles the subsurface may be obtained (Figure 2-2).



Figure 2-1 Ray paths and resulting synthetic seismogram. The background P-wave velocity and Poisson's ratio are 6000 m/s and 1.73, respectively. The reflectors are modelled as fracture zones having a P-wave velocity of 5000 m/s and a Poisson's ratio of 2.

Although the migrated image in Figure 2-2 resembles the sub-surface there are some important differences. First, the dipping reflectors are not necessarily imaged below the points where the shots were fired, but are observed most clearly where the interfaces are at right angles to the source. This is because reflected waves obey Fermat's principle of taking the ray path which gives the shortest time of propagation. In order to image

steeply dipping interfaces then requires that long profiles are shot even if the area of interest is relatively small. Secondly, there are artefacts in the stacked section between 600 m to 800m depth on the right hand side of the migrated image (Figure 2-2). These are P- to S- converted wave reflections which are not handled properly even when prestack migration is applied. In principle it is possible to migrate these waves correctly, but on real data it is difficult to discriminate between which waves are which when only one component of motion is recorded. Finally, note that exactly the same image would have been obtained if the subsurface geometry was rotated at an angle perpendicular to the direction of profile. That is, from 2D lines it is not possible to determine from what direction the reflected events are arriving at, a sub-horizontal event could just as well originate from a near-vertical interface from out of the plane of the profile.



Figure 2-2 Reflector model as in Figure 2-1 and the results from pre-stack migration and stacking 10 shots to obtain the image on the left. The position of the shots used in the migration are shown by inverted triangles along the top of the section.

3 Reflection coefficients

In elastic media the strength of a reflected wave will be dependent upon the angle of incidence of the incident wave. In addition, a P-wave which impinges on an interface at non-normal angles of incidence will give rise to reflected S-waves as well as P-waves. The strength of these reflected waves (the reflection coefficients) are dependent upon the P-wave velocity (Vp), the S-wave velocity (Vs), and the density (ρ) of the media above and below the interface. If the reflection is due to lithological contrasts in the two media there will be a tendency for the P-wave energy to increase with increasing angle of incidence (Figure 3-1) and for the P- to S-wave energy to gradually increase in

magnitude. In contrast, if the reflections is from a fluid filled fracture zone the P-energy will be expected to decrease with angle of incidence and the P- to S-wave energy to increase rapidly (Figure 3-2). The greater the Vp/Vs ratio in the fracture zone the more pronounced this effect will be.



Figure 3-1 Reflection coefficient vs. angle of incidence for a granitic/mafic interface.



Figure 3-2 Reflection coefficient vs. angle of incidence for a granitic in-tact/fracture zone interface.

4 SG-4 example

4.1 Data acquisition

The SG-4 borehole is located in the Tagil Synform of the Middle Urals in Russia and had reached a depth of 5354 m as of August 1995. The final depth is targeted to 15000 m. The penetrated rocks are of island-arc origin and have been proven to contain clear strong reflectors (Juhlin et al., 1997). A particularly strong reflector is imaged at about 3000 m depth close to where a seismic line crosses the SG-4 borehole. The geological structure strikes mainly north-south and surface observations along with seismic data indicate that lithological boundaries and thrust faults dip at about 30-50° to the east. However, near-vertical fracture zones cut at angles across the geological strike. Vertical seismic profile (VSP) data have been acquired to image the surface seismic reflectors and determine the source of reflectivity. Data were acquired in two campaigns in the cased part of the borehole within the depth interval 520 m to 3940 m with shots offset from the wellhead by as much as 1840 m. The presence of dipping geological structure and sub-vertical faults is consistent with the complex wavefields recorded on the VSP data.

4.2 Data processing and interpretation

Downgoing waves are strong in VSP data and generally need to be removed before clear upoing or reflected waves can be observed. On shots offset greater than 400 m to the north of the wellhead a clear upoing reflected wave is observed (Figure 4-1). Processing steps were kept to a minimum and include bandpass filtering (10-20-60-90 Hz), removal of downgoing P-waves, removal of downgoing S-waves and coherency filtering. Other shots record reflected waves from steep interfaces (dips up 85°).

The apparent velocity of the reflected wave in Figure 4-1 is too low for it to be a Pwave which implies that it must be either a reflected S-wave or a converted P- to S-wave reflected wave. Synthetic data were generated to match the traveltimes and amplitudes of the reflected event (Figure 4-2). Excellent traveltime agreement between the synthetic and real data is achieved for both the reflected P-wave arrival (the earlier event arriving at 0.65 s at 1120 m and at 0.56 s at 2120 m) and the reflected S-wave arrival (the later event arriving at 0.9 s at 1120 m and at 0.61 s at 2120 m). The strong event on the N-S component on the real data which arrives about 0.1 s after the first reflected S-wave is probably a multiply reflected wave. It is difficult to judge the amplitude agreement of the reflected waves since in the real data there are numerous additional reflected waves which interfere with the main events. However, the qualitative amplitude agreement is good. If the reflector is modelled as a mafic interface then the traveltime agreement is the same since no changes were made in layer 1, however, the qualitative amplitude agreement is poorer. In addition, polarity studies indicate the reflected S-wave to be from a negative impedance interface. These observations strongly suggest that the reflected arrivals are from a fracture zone.



Figure 4-1 Three component data from the SG-4 borehole showing a clear dipping Pto S- wave converted reflection. The source was offset from the wellhead by 31 m to the east and 839 m to the north.



Figure 4-2 Synthetic data from simple modelling of the P- to S-wave converted event in Figure 4-1. The model consists of an interface dipping 30° to the east, striking N-S, and intersecting the borehole at 2900 m. The elastic parameters were Vp=6100 m/s, Vs=3500 m/s, $\rho=2700 \text{ kg/m}^3$ for layer 1 and Vp=5500 m/s, Vs=2500 m/s, $\rho=2500 \text{ kg/m}^3$ for layer 2.

5 Ävrö example

5.1 Data acquisition

As part of the Swedish Nuclear Waste Management Companay's (SKB) research program, reflection seismic measurements were carried out on the island of Ävrö in South-eastern Sweden. Ävrö island is situated just to the Southeast of Äspö island, the location of the Äspö Hard Rock Laboratory (Hammarstöm and Olsson, 1996). The main objectives of the seismic measurements were (1) to test the method for future site investigations in other areas (2) to map a known hydraulically conductive fracture zone that intersects a borehole between 400 and 600 m measured depth and (3) to add to the database of reflection seismic studies on the shallow crystalline crust in Sweden. In order to obtain 3D control of the known fracture zone two ~1 km long crossing high resolution seismic lines were shot (Juhlin and Palm, 1997). The W-E one (Line 1) had a station spacing of 5 m on average and the N-S one (Line 2) had a station spacing of 10 m on average (Figure 5-1). The profiles cross one another close to the ~740 m deep borehole KAV01. Shot and geophone points were placed, to the greatest extent possible, on bedrock. Drillers of shotholes were instructed to drill at the closest suitable location to a staked point where bedrock outcrop was present, but not further than 1 m parallel and 2 m perpendicular to the profile from the staked point. If no bedrock was found within this area the hole was drilled at the staked point. Geophone holes (8 mm diameter, 50 mm deep) were later drilled following the same instructions, but were not necessarily drilled close to the shotpoints. Weather conditions were excellent during the one week period it took to acquire the data.



Figure 5-1 Location of seismic profiles on Ävrö (crossing at the KAV01 borehole), the majordipping fracture zones which are observed on them (A, B and C) and the major geophysical anomalies present in the area.



Figure 5-2 N-S and W-E seismic profiles merged where they cross and viewed from the NW (left) and SE (right).

5.2 Data processing and interpretation

Standard processing was applied to the two seismic lines including DMO. After merging the two lines where they cross (Figure 5-2) several clear reflections are observed (labelled A, B and C). Event A dips at an angle to both profiles and strikes about 60° to Line 2. It projects to the surface along the Southeast coast of Ävrö. Event B on Line 1 appears to be sub-horizontal, but has a true dip to the South and projects to the surface close to CDP 1 on Line 2. Event C dips steeply to the East and projects to the surface close to CDP 60 on Line 1. Other sub-horizontal events away from the intersection point may also come from out of the plane, but this cannot be proven without further data acquisition.

Events A, B and C on Lines 1 and 2 can be projected to the surface (Figure 5-1). Their strike and dip are constrained by their apparent dip on Lines 1 and 2. Reflector A projects to the surface Southeast of Ävrö and dips ~50° to the Northwest. It is observed on both seismic lines, however, the KAV01 borehole does not penetrate it. If the hole were to be deepened, reflector A would be expected to be penetrated at about 1000 m depth. Reflectors B and C strike approximately perpendicular to Line 2 and Line 1, respectively, and can, therefore, be subjected to 2D migration. After migration, reflector B dips at about 35° to the South and the top of it intersects the borehole at about 400 m. Reflector C is much steeper, about 60°, and the point where it intersects the borehole is not clearly imaged. However, the projection of the reflector downwards implies the

top of it intersects the borehole somewhat below 500 m. The hydraulic conductivity in borehole KAV01 increases significantly between 400 and 600 m. It is probable that this increase is due in part to reflectors B and C intersecting the borehole in this depth interval.

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AN OPTIMIZATION PROCEDURE FOR BOREHOLE EMPLACEMENT IN FRACTURED MEDIA

Daniel Billaux

Itasca Consultants S.A., 40 avenue Guy de Collongue, F 69130 Ecully, France

Frédéric Guérin Krebs, 8 rue J.P. Timbaud, F 78180 Saint Quentin en Yvelines, France

Abstract

Specifying the position and orientation of « the next borehole(s) » in a fractured medium, from prior incomplete knowledge of the fracture field and depending on the objectives assigned to this new borehole(s), is a crucial point in the iterative process of site characterization. The work described here explicitly includes site knowledge and specific objectives in a tractable procedure that checks possible borehole characteristics, and rates all trial boreholes according to their compliance with objectives.

The procedure is based on the following ideas : Firstly, the optimization problem is strongly constrained, since feasible borehole head locations and borehole dips are generally limited. Secondly, a borehole is an « access point » to the fracture network. Finally, when performing a flow or tracer test, the information obtained through the monitoring system will be best if this system detects the largest possible share of the flow induced by the test, and if it cuts the most « interesting » flow paths.

The optimization is carried out in four steps. 1) All possible borehole configurations are defined and stored. Typically, several hundred possible boreholes are created. Existing boreholes are also specified. 2) Stochastic fracture networks reproducing known site characteristics are generated. 3) A purely geometrical rating of all boreholes is used to select the « geometrically best » boreholes or groups of boreholes. 4) Among the boreholes selected by the geometrical rating, the best one(s) is chosen by simulating the experiment for which it will be used and checking flowrates through possible boreholes.

This method is applied to study the emplacement of a set of five monitoring boreholes prior to the sinking of a shaft for a planned underground laboratory in a granite massif in France (« Vienne site »). Twelve geometrical parameters are considered for each possible borehole. A detailed statistical study helps decide on the shape of a minimization function. This is then used to select 10 « geometrically best » sets of 5 boreholes. The flowrates induced by the shaft sinking are then simulated. By comparing the flowrates passing through all the tentative boreholes, we are able to give recommendations on the most suited setup.

1 Introduction

This work was commissioned by ANDRA in the framework of the study of a possible Underground Research Laboratory in granite in the Vienne area. The sinking of the planned access shaft will cause an hydrogeological perturbation of the volume it will cut. Following the effect of this perturbation by means of an appropriate array of monitoring boreholes will yield useful information about the properties of the hydrogeological system.

Laying the monitoring boreholes is an optimization problem, and is made difficult by the scarcity of our prior knowledge of the site. The objective of this work is to perform such an optimization, using our uncomplete knowledge to constrain the geometry of the group of boreholes. Our guiding principle is to formalize (i.e. « to translate into mathematical terms ») some aspects of the geological and hydrogeological reasonning. In this way, a tractable borehole selection procedure is developed, which includes both site knowledge and the specific objectives assigned to the borehole or group of boreholes.

Note that we are interested here by the « large fractures » network, with scales of several hundred meters at least.

2 Outline of the procedure

2.1 Rationale

We first note that site characterization is an iterative process : we are not defining all boreholes *a priori*, but are working back and forth between field phases and interpretation/modelling stages. Decisions on borehole emplacement will be more precise, and therefore the borehole array will be more efficient, if the successive phases and shorter and more numerous.

Also, in order to enable a rigorous process, the objective of the characterization campaign must be precisely defined : « detect the large flow paths network », « knowledge of the hydrogeological interaction with overlaying sedimentary layers », « determination of the large scale specific storage » for example. More than one objective may be pursued, as long as they are clearly prioritized.

The methodology we present here is oriented towards the first of the objectives listed above (« detect the large flow paths network »). The basic principles can easily be used to develop a procedure aimed at other objectives.

We start from the following observations :

• The numbers, positions and orientations of the future borehole are severely limited by several constraints : work-schedule, possibilities for installing boring machines, minimum borehole dip, presence of laboratory drifts that must be avoided. It is therefore possible to systematically study all feasible boreholes, with a fine enough mesh, as long as the checks to be performed on each « possible borehole » are simple.

- The « quality » of a given borehole is the « amount of information », in terms of fracture and network properties, to which this borehole gives access. From a strictly geometrical viewpoint, the borehole quality is higher if it has more connections with the network we are trying to explore. This explains why we try to drill boreholes the least parallel possible to the main orientations of fracture planes. This thought process may be continued one step further : a given intersection between a borehole and a fracture is all more the interesting that it provides, through this fracture, connections to other conducting elements which will be able to influence measurements in this borehole, and therefore be possibly detected.
- It is mostly through interference tests that the large fractures network may be characterized. During such tests (for example the « pumping test » due to sinking the access shaft), measurements by the monitoring system will contain all the more information if they integrate the largest possible share of the disturbance. One may ask the following question : out of the x cubic meters pumped into or out of the environment, how many can be detected by the monitoring system, and thus contribute to our knowledge of the network ?

2.2 Steps of the optimization process

We start from the set of all possible borehole arrangements, generate fracture networks integrating the known properties of the site, select several groups of boreholes based on geometrical rating, and then chose between these groups by modelling the hydraulic disturbance created by the access drift and computing what flow rates are detected.

2.2.1 Building the model

This consists of two operations : defining possible boreholes, then generating fracture networks. Possible boreholes are specified by the positions of the boring rigs, orientation (dip, dip direction) intervals, their length, and the depth of the sediment/granite contact, above which a borehole is not taken into account. Figure 2.1 shows the set of 845 possible boreholes specified for the Vienne study.

Fractures are considered as discs, with orientations and linear densities (i.e. numbers of fractures per meter of borehole) given by the existing borehole information. From the few boreholes already existing and from their study by structural geologists, we can deduce the orientation statistics and relative weights of five fracture sets. We have very little information about fracture size, besides the fact that from interference tests the network is probably connected. We use a law with a mean radius of 500 m and a small standard deviation, producing networks of average connectivity. Fractures are generated in a 3 km by 3 km by 1 km high box, centred on the planned position for the access drift. Disc centres have random positions (Poisson point process) in the generation volume. Two boreholes have already drilled in this volume, and seven fractures were detected. The fracture generation process is conditioned on these seven known fractures : their exact positions and orientations are reproduced, and no other « random » fracture crosses these boreholes.



Figure 2-1 All possible boreholes for the Vienne study

2.2.2 <u>Geometrical sort</u>

The aim of the geometrical sort is to obtain a set of groups of boreholes (here ten fiveboreholes groups) with an optimum quality in terms of geometry. The procedure assigns to each borehole a mark depending on its connections with the fracture network, and on its connection through the fracture network with the access shaft and other boreholes.

A large number (50 to 200) of realizations of the fracture network is generated. For each trial borehole and for each realization, several parameters are computed. For each borehole, the mean value of a parameter for all realizations is used to assign a mark between 0.5 and 1.2 in general (for some special cases, we may want to formally discard a borehole and therefore apply a mark of 0). The final mark of the borehole is the product of these various individual marks.

The following parameters are computed and produce a mark (figures 2.2 and 2.3)

- Borehole dip.
- Distance to planned underground laboratory galleries.
- Number of fractures cut by the borehole.
- Number of fracture intersections reachable from the borehole.
- Percent of the number of realizations for which there exists a connection to a given « origin borehole ».
- Length of the shortest path along the network to an « origin borehole ».
- Angle with any already chosen borehole on the same rig.
- Number of boreholes already chosen on the rig.



Number of fractures cut by the borehole

Number of fracture intersections to which the borehole gives access



Figure 2-2 Geometrical parameters for the sort.



Number of boreholes on the rig



Angle with another borehole on the same rig



Figure 2-3 Geometrical parameters for the sort.

The two parameters referring to an « origin borehole » are in fact computed several times, yielding one mark each time. « Origin boreholes » are the following :

- The access shaft.
- Existing boreholes in the volume of interest here two boreholes named CHA112 and CHA212.
- If one or more borehole have already been chosen in the group of boreholes being currently put together, these already chosen boreholes.

For each parameter, we first perform a statistical study, in order to chose the grading scale we will use for this parameter. A sensibility study is performed to ensure that small changes in the grading system have a small effect on the outcome of the procedure. The correlations between parameters are also examined, to check eventual redundancies.

The grading scales are chosen to reflect as closely as possible the thinking of the geologist and hydrogeologist, and may be described in terms of the « ideal borehole »: dips over 60°; minimum distance of 10 m to planned galleries; cuts many fractures, with many fracture intersections; high probability of connection with the access shaft, existing or planned boreholes; hydraulic paths not too long towards the access shaft, existing or planned boreholes - also, hydraulic paths no too short towards other planned boreholes; minimum angle of 30° with another borehole on the same rig; maximum of two boreholes from one rig

The treatment is first performed in order to chose the first borehole in the first group. These grades only take into account the network properties and *a priori* chosen constraints. We name them « intrinsic marks ». We then recompute grades for all the boreholes, taking into account the presence of the first chosen borehole, and use these new grades to chose the second borehole. By repeating this procedure, we can chose all the boreholes in the first group.

In order to obtain the first borehole in a new group, we come back to the intrinsic marks, discarding boreholes already chosen as heads of a previous group. The following boreholes in the group are then chosen in the same manner as before.

2.2.3 Hydrogeological sort

This final step discriminates between the groups of boreholes selected by the geometrical sort. For each realization of the network, the planned test (or tests) is simulated. For the « Vienne » site, we model the sinking of the access shaft, equivalent to a large scale pumping test. For each selected borehole, flowrates through its intersections with fractures are summed. The « best » group of boreholes is then the one detecting, on the average, the largest share of the flowrate pumped from the shaft.

3 Results and conclusion

In order to help visualize parameter behaviour, we perform an interpolation of the intrinsic mark for each borehole, using Schmidt diagrams (lower hemisphere) as a mapping support. One interpolation is done for each position of the rig. This interpolation is a krigeing based on a simple linear model.

Figure 3.1 shows the five Schmidt diagrams corresponding to the five possible rig positions, and the arrangement of the diagrams on the figure roughly reproduces the relative positions of the five rigs. On these diagrams, each cross corresponds to one possible borehole (smallest dip 40°, south-dipping boreholes at the bottom of a diagram). The isolines represent the intrinsic mark, normalized to a maximum of 10.

Figure 3.2 shows all the boreholes selected in at least one group by the geometrical sort. The first borehole for all 10 groups is always on rig PF25, with a 60° or 70° dip.

The main borehole directions are to the east and north, which is coherent with the main fracture dip directions to the west an south. However, the influence of relative positions of the rigs can also be seen : PF24, being too far from the shaft, has no borehole selected, and in PF22 the weight of the « path length » parameter forces the selection of west-trending boreholes.

The flow simulations yield for the ten groups of boreholes average total flowrates detected (over 200 realizations) between 4 % and 10 % of the flowrate extracted from the shaft. The \ll best \gg group from these simulations is outlined in figure 3.2.

The procedure was developed with flexibility as an objective. This means that changing the parameters depending on the specific objectives pursued is simple, as long as the criterions can be stated geometrically. It can also be used iteratively, since it is geared towards taking successively into account existing or already chosen boreholes.

The use of the method described here should obviously never be of the « black box » type. Its main advantage is to be a tool for understanding, by which the geologist and the engineer can check how the priorities they chose affect the choice of borehole positions. In the framework or radioactive waste disposal studies, the decision-making process can thus be formalized and made more tractable.





Figure 3-1 Schmidt diagrams (lower hemisphere) of intrinsic marks normalized to 10.


Figure 3-2 Boreholes selected in at least one group by the geometrical sort. « Best » boreholes from the hydrogeological sort are outlined.

DESIGN CONSIDERATIONS FOR THE ACQUISITION OF HYDROCHEMICAL DATA FROM DEEP BOREHOLES

Ross McCartney, Peter Ledingham

GeoScience Limited, Falmouth, United Kingdom.

Abstract

Deep (>300 m) subsurface hydrochemical data are important components of geological investigations of potential radioactive waste disposal sites. These data can be interpreted to yield information that supports conceptual hydrogeological models, constrains palaeohydrogeological evolution and characterises subsurface hydrochemical conditions of a site. The most important sources of these data are the analyses of groundwater samples collected during extraction tests performed in boreholes either during drilling or after drilling has been completed. To maximise the information obtained from their interpretation, the quality and quantity of hydrochemical data obtained should be such that they are representative of the compositions of the in-situ groundwaters, the in-situ location of all groundwaters should be known, and the key trends in groundwater compositions should be identifiable from the data set.

The design of deep borehole-based hydrochemical data acquisition programmes to meet such objectives is a complex task. It is useful to simplify the design process by focusing attention on those activities and parameters that are most likely to affect the quality and quantity of hydrochemical data obtained from the final implemented design. In this paper we examine those design parameters associated with drilling (cutting method, drilling fluids, flushing method, drill string and bottomhole assembly), fluid extraction testing (timing, test tools, fluid extraction method), sampling (sampling locations, timing of sampling, numbers of samples, sample collection methods), and sample analysis (analytical precision and accuracy, location and timing of analyses) activities. For each parameter we discuss the design options available, and identify those with features that are most likely to be beneficial or detrimental to the quality and quantity of hydrochemical data.

Preferred design options have been identified where possible. However, each investigation will have a number of external constraints associated with it arising from either the investigation itself, the site or available technology. As a result, depending on the circumstances of each investigation, it may not be possible to include all the preferred design options into a final design.

1. Introduction

An important objective of geological investigations of potential radioactive waste disposal sites is the collection of hydrochemical (groundwater composition) data from deep (>300 m) locations at the site. The interpretation of these data can be used to yield information that supports conceptual hydrogeological models (eg Nirex, 1998a), constrains palaeohydrogeological evolution (eg Fontes, 1994) and characterises subsurface hydrochemical conditions of a site (eg Pearson and Scholtis, 1993).

The principal sources of these data, and the subject of this paper, are analyses of groundwater samples collected during extraction tests performed in boreholes either during drilling or after drilling has been completed. To maximise the information obtained from interpretation, the quality and quantity of the hydrochemical data should be such that they are representative of the compositions of the in-situ groundwaters, the in-situ location of all groundwaters should be known, and the key trends in groundwater compositions should be identifiable from the data set. The quality and quantity of hydrochemical data obtained are largely determined by the activities associated with the drilling of the borehole, extraction of groundwater from the formation, and collection and analysis of groundwater samples (primary activities).

The design of primary activities to obtain hydrochemical data will normally be constrained by a number of factors. These may be associated with the investigation itself (eg financial, programme, priorities placed on the acquisition of different data, limitations on borehole locations, etc), the site (eg local geological conditions, groundwater compositions, etc), or they may be of a technical nature (eg availability of equipment, techniques, methods, etc). Under such circumstances, the designer needs to consider which design parameters will most influence the quality and quantity of hydrochemical data obtained and what options are available for each parameter. The designer can then choose options that will best provide the data required given the constraints.

Based on our experiences on the UK Nirex investigation at Sellafield, and building on the experiences of other earlier investigations(eg Bottomley et al., 1984; Smellie et al., 1985; Haug, 1985; Smellie and Wikberg, 1991; Ross and Gascoyne, 1995), in this paper we will identify the key design parameters for the primary activities and discuss design options available for each parameter. For each option, we will also identify those with features that are most likely to be beneficial or detrimental to the quality and quantity of hydrochemical data obtained, and where possible, we will identify those design options that are preferred for deep borehole-based hydrochemical data acquisition programmes.

2. Drilling Design

2.1. Cutting Method

Given the typical depths of investigation boreholes, two cutting techniques may be considered: rotary or percussive drilling, and coring. Both methods may provide similar penetration rates but coring is preferable because the finer cuttings produced allows lighter drilling fluids to be used. As discussed below, this minimises borehole pressures, and hence contamination of the groundwater with drilling fluid. Collection of core is beneficial to water-rock interaction studies, may allow core pore fluid data to be obtained and helps provide information about the condition of the rock in the proposed fluid extraction test interval (eg the location of potential flowing features and suitable packer seats).

2.2. Drill fluids and flushing method

Drilling fluid losses to the host rock are most likely to occur at any points where the pressure in the borehole exceeds that in the formation. The highest borehole pressures occur at the drill bit where some losses are inevitable. Losses may be reduced using drilling fluid additives or by keeping borehole pressures as low as possible. The latter can be accomplished by the use of low density fluids or artifical lifting (eg gas injection).

Constituents in groundwaters affected by drilling fluids can be categorised as being affected by either mixing-type contamination or reaction-type contamination (McCartney and Solbé, in prep.). Reaction-type contamination may result from a variety of interactions involving the drilling fluid, groundwater, drilling fluid/groundwater mixtures, formation minerals, secondary reaction products and drilling fluid debris (see Figure 2-1). A number of studies have identified the potential for drilling fluid materials to be retained in the formation after they have been lost (eg Graham and Johnson, 1991). Baeyens and Bradbury (1991) have shown how even 'pure' groundwaters can have their compositions modified during transport to the borehole through reactions with drilling fluid losses (eg bentonites, polymers, etc) should be avoided where possible because although mixing-type contamination effects can be corrected (see below), drilling fluid-groundwater-formation mineral reactions are poorly understood. Thus, it is difficult to attempt to make corrections to reaction-type contaminated groundwater composition data. The use of complex drilling fluids may also lead to plugging of fractures.

Low density drilling fluids may include either air or low salinity water. In deeper (>250m) or inclined holes the cuttings lifting characteristics of air can be poor (eg Smellie and Wikberg, 1991) which can jeopardise the drilling of the hole itself. Use of air as the drilling fluid can also lead to oxidation of the formation and groundwaters, particularly at greater depths where air injection pressures are high (Bottomley et al., 1984; Smellie and Wikberg, 1991). A compromise drilling fluid would be low salinity water which has better lifting characteristics than air and its interactions with groundwaters and formation minerals are better understood than drilling fluids with additives. It is preferable to choose a low salinity water with a composition that will



least affect the groundwater composition by mixing or reaction.

Figure 2-1 Schematic representation of interactions occurring between drilling fluids and groundwaters following losses of drilling fluid to the formation and during their subsequent extraction.

Two methods have been used to artificially reduce borehole pressures during drilling: normal (eg Almén and Zellman, 1991) and reverse (eg Ljunggren, 1993) air-assisted drilling fluid circulation. Although drilling fluid contamination of groundwaters is minimised with the normal method, this effect is not avoided (Nirex, 1998b). There are practical limitations on the use of the reverse method (eg fluid flow from the formation needs to be fairly continuous and uniform; Ljunggren, op. cit.). With both methods there is an increased risk of disturbing the initial distribution of groundwaters due to the net inflow of groundwater to the borehole during drilling. There is also a risk of cross-flow contamination of sections of the formation during breaks in drilling. However, both risks can be minimised by using drill-and-test methods (see below), continuous drawdown below minimum formation pressure and surface read-out downhole pressure monitoring. With both methods, by monitoring the composition of drilling fluid produced from the borehole, the location of significant inflows of groundwater to the borehole may be identified and can aid the selection of fluid extraction test zones.

As drilling fluid contamination of groundwaters is to be expected, the drilling fluid should include an inert tracer. The presence of inert tracer in a sample can demonstrate the presence of mixing-type drilling fluid contamination which itself identifies the potential for reaction-type contamination. Control of the inert tracer and drilling fluid composition and collection and analysis of drilling fluid samples during drilling will allow the groundwater compositions of those constituents only affected by mixing with drilling fluids to be estimated (eg ³H, Cl, Br, etc; McCartney and Solbé, in prep.). Such data will also assist with the deconvolution of drilling fluid/groundwater reaction effects. Graham and Johnson (1991) have suggested the use of 'reactive' tracers in

drilling fluids to trace reaction-type contamination although such a technique would be limited to those constituents that undergo similar reactions to the tracers used. Where groundwater flows into the borehole during drilling, as with air-assisted methods, control of the drilling fluid and tracer composition can be difficult. If water supply and disposal are not limited, these problems can be avoided through the use of open-loop drilling fluid circulation (ie drilling fluid is not re-circulated into the borehole).

2.3. Drillstring and Bottom Hole Assembly

Core may be recovered during drilling either conventionally where the core barrel is removed with the drillstring or by wireline recovery, where the core can be recovered without removing the drillstring. Wireline recovery minimises movement of the drill string in and out of the borehole and therefore reduces the potential for drilling fluid invasion of the formation and for cross-flow contamination due to surging and suction effects.

Debris from the materials from which the drillstring, downhole tools and bits are made (including lubricants) may be deposited on the borehole walls, settle to the bottom of the borehole or may be carried into the formation with drilling fluids. Groundwaters entering the borehole during extraction testing may react with this debris. As a general principle, any drilling related materials should be tested for their potential reactivity with the anticipated groundwaters before drilling proceeds. Drilling equipment should be selected so as to minimise the potential impact on chemical constituents of interest. The same can be said of all equipment used during testing, sampling and analysis. Consideration should be given to the use of less reactive materials such as Stainless steel, PVC or teflon coated equipment, solid lubricating materials such as PTFE, etc.

2.4. Hole size

Small diameter holes are preferable because the annulus between the borehole wall and drill string is likely to be small. This allows high fluid return velocities to be achieved, which assists the removal of cuttings and improves the performance of lower density drilling fluids. There is also a smaller volume of drilling fluid in circulation which simplifies water supply and disposal in open-loop circulation systems. A small hole size will also reduce the volume of borehole associated with a section to be tested (see below).

3. Extraction tests

3.1. Timing

There are two general approaches to the timing of testing in relation to drilling activities. Testing may either take place at progressively greater depths as the borehole is drilled (drill-and-test method) or a relatively large section of the borehole will be drilled and subsequently tested (drill-then-test method). The former approach is preferable with respect to the quality of groundwater samples because the longer a section of borehole remains untested, the greater the potential for drilling fluid contamination of

groundwaters and the associated disturbance of the groundwater distribution adjacent to the borehole. With either approach, extended breaks during or after drilling may increase the risk of cross-flow contamination via the open hole. The latter can be avoided through monitoring the formation pressure with depth, maintaining a drawdown on the borehole greater than the lowest formation pressure, and/or through the separation of active zones by packers.

The section of borehole to be tested should contain fractures or porous formations capable of having fluids extracted from them with the equipment and extraction methods available if groundwater samples are to be collected. Production logs (electrical conductivity, temperature, flow) used in conjunction with geophysical logs on borehole sections are the preferred method of identifying such features. For the drill-test approach, frequent production logging may be impractical. In such cases, changes in drilling parameters (eg drilling fluid losses and gains) or identification of potential flowing features in core can be useful but are less reliable.

3.2. Test tools

Testing a small section of the borehole will minimise the possibility of sampling more than one compositional type of groundwater (ie artificially mixing the groundwaters and disturbing the original groundwater distribution). This can be achieved using straddlepackers positioned around the zone to be tested or, if the test zone is at the bottom of the borehole, a single packer located just above the zone to be tested. The packers may be set via a surface inflation line or by rotation. Inflation by pressurisation of the test string with water can result in contamination of groundwater samples during short duration, lower flow rate extraction tests when downhole samplers need to be used (see below). The inclusion of a shut-in valve in the test tools provides further sampling opportunities (see below) and allows the formation pressure to be measured. The risk of groundwater contamination through packer leakage can be minimised through the use of guard packers and selection of packer seating zones using information from core or televiewer logs. Packer leakage can be detected by monitoring the pressure in the guard zones and test sections. Surface readout of pressure allows a more rapid response to detected problems. The reduction of dead volumes between the packers will minimise diffusive contamination of groundwater samples. Dispersive contamination will also be minimised where several minor fractures intersect the borehole in addition to the major fracture. By limiting the test string diameter, groundwater samples will be more quickly produced at the surface, minimising groundwater contact with the test string.

3.3. Fluid extraction method

If the formation is not artesian, the fluid can be extracted from the formation and borehole using gas-lift (eg air, nitrogen), mechanical bailing devices (eg swabbing, bailers) or submersible pumps. Greater rates of extraction tend to be achieved using gaslifts and high capacity pumps. However, if samples are to be collected at the surface during extraction tests (see below), each of the methods may affect the groundwater composition. For example, gas-lifting strips the groundwaters of dissolved gases, contaminates them with the gas used for lifting and can warm or cool the groundwaters depending on the gas and groundwater temperatures. Air contamination, pressure loss and temperature change are common problems with groundwaters extracted by swabbing and bailing. With this method, 'drain back' of fluid into the test string can result in air contamination of samples subsequently collected downhole (Ross and Gascoyne, 1995). Gas loss through de-pressurisation and temperature changes are common in artesian or pumped groundwater samples.

Each extraction method results in a decrease in test section pressure relative to that in the formation (ie a pressure drawdown). Increased drawdown on the test section increases the risk of packer leakage (sample contamination) and borehole breakout (potential loss of borehole). Similarly, it increases the risk of disturbing the natural distribution of groundwaters in the formation. In extreme cases, reduction of formation pressure may lead to outgassing and changes in groundwater composition in the formation. It is therefore preferable to limit drawdowns so that they do not exceed the in-situ gas pressure in the groundwaters.

4. Sampling

4.1. Sampling locations

Groundwater samples can be collected from four generic locations during extraction tests; downhole in wireline samplers in the test string just above the test section, downhole in samplers within the test section tools, at the surface next to the wellhead, and from the test string at the surface as it is removed from the borehole at the end of the test. Downhole wireline samplers provide the best quality samples if they are obtained below any disturbances caused by the extraction method. They have limited contact time with downhole equipment and may also be the only method of collection under low flow rate extraction conditions. Samplers are available that can maintain the samples under pressure up to the point of sample analysis. However, sample size is limited (typically less than 5 litres) making multiple sampling runs necessary. The act of running the samplers into the test string can lead to artificial mixing of the fluids in the test string which can be problematic in low flow rate extraction tests. Large samples can be obtained from the surface or test string without contacting the atmosphere if degassing, de-pressurisation or extended contact with the test string is not problematic for the constituent of interest. All samples are affected by temperature changes during transport out of the formation although, if the temperature changes are measured, any changes in groundwater composition (eg pH) can be calculated and corrected for (eg Pearson et al., 1989).

4.2. Timing of sampling, numbers of samples and sample collection methods

A groundwater 'sample' is often made up of a set of samples collected at approximately the same time but from different locations. Analyses for each constituent are performed on those samples for which the best quality data can be obtained. There are two general approaches that are adopted with respect to the timing of collection of sample sets. A series of sample sets may be collected over time during the test (time series sets) or one or more sample sets can be collected at the end of the test (end of test sets). Time series sets can be used for extrapolating the groundwater composition where a drilling fluid tracer is used. This can keep test durations short and minimises disturbance to the groundwater distribution but extrapolation techniques have their limitations (see above). The end of test approach seeks to obtain what can be considered to be pure groundwater samples (ie when, for the constituents of interest, drilling fluid contamination is negligible). Test durations tend to be longer and the risk of disturbance to the groundwater distribution is increased. In addition, even when drilling fluid tracer levels are low, drilling fluid contamination of samples may still occur (eg Baeyens and Bradbury, 1991). Alternative methods of assessing drilling fluid contamination clean-up (eg achievement of a steady extracted fluid composition or extraction of pre-calculated volumes) can be misleading (Graham and Johnson, 1991).

Alteration or contamination of samples during collection and prior to analysis can be minimised through judicious selection of sample collection methods. This includes immediate post-collection treatment of samples (eg transfer of samples between vessels, addition of preservatives, pre-concentration, filtration, storage, etc).

5. Sample Analysis

5.1. Analytical precision and accuracy

Although short term precision can be measured for quality control purposes, the most meaningful measure of analytical precision is long term precision determined by analysis of an 'internal standard' with each batch of analyses (Taylor, 1987). As well as being a quality control tool it allows confident comparison of data obtained throughout a site investigation. Internal standards should preferably have compositions similar to the samples being analysed.

Accuracy of the chosen analytical methods may be assessed through their use to measure (a) international reference standards, (b) samples used in inter-laboratory analysis comparison schemes, (c) laboratory prepared reference standards, or (d) spiked samples (Taylor, 1987). Again, preferably these should have compositions similar to the samples collected from the site. This is rarely the case for the former two options. For the latter two options, demonstration of accuracy will normally be retrospective. In any event, assessment of the accuracy of measurements will require expert judgement.

5.2. Location and timing of analyses

Ideally, samples should be analysed in a location that (a) minimises alteration or contamination of the sample after collection, (b) is suitable to the timing of use of the analytical results and (c) is appropriate to the analytical method. The four general analytical locations are: downhole in the test string or test tools, at the wellhead, in an on-site laboratory or in an off-site laboratory. Examples of constituents that may be measured downhole are Eh and pH (eg Almén et al., 1986), each of which may change during transport to the surface during extraction tests due to interaction with test string and the atmosphere, and temperature and pressure changes. These constituents and others (eg electrical conductivity, dissolved oxygen, etc) are also often measured at the wellhead (eg Almén et al., 1986). Due to equipment and calibration problems, there is some debate about whether downhole Eh and pH measurements are better than the

wellhead measurements (Whitaker et al., 1994). Where sample contamination or alteration (eg microbial activity, atmospheric effects) may affect particular constituents (eg alkalinity, Fe^{2+} , Fe^{3+} , NO_3 , etc) soon after collection or where the data is needed for decision-making purposes (eg drilling fluid tracer), analyses are best performed on-site soon after sample collection. Where it is possible to maintain samples in a stable condition for particular constituents for a relatively long period, analysis for these constituents may be performed on-site or off-site some time after collection.

6. Conclusions

The design of activities to acquire hydrochemical data from boreholes is a complicated task. However, this task can be simplified if (a) those design parameters that are most likely to affect the quality and quantity of hydrochemical data obtained can be identified, (b) the design options under each parameter can be identified, and (c) the potential impact of these different options on the data can be assessed. This information can allow the designer to focus on design solutions that best match the external constraints associated with the investigation itself, the site and available technology.

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CHARACTERISATION OF DEEP GROUNDWATERS AT OLKILUOTO AND HÄSTHOLMEN (FINLAND) - RECENT RESULTS WITH PAVE, A SAMPLING EQUIPMENT MAINTAINING THE IN SITU-PRESSURE.

Paula Ruotsalainen Fintact Oy, Helsinki, Finland

Margit Snellman Posiva Oy, Helsinki, Finland

Abstract

The Finnish bedrock has been investigated since 1987 for final disposal of spent nuclear fuel. Saline (TDS>10 g/l) groundwaters have been observed at Olkiluoto and Hästholmen, two of the presently studied four sites. The new sampling equipment, PAVE, keeps deep groundwater samples in the in situ-pressure. The pressure vessels of the PAVE sampling system are divided into two parts by a movable, o-ring sealed piston. As the pressure compartment of the pressure vessel is filled with argon gas, the piston moves up. Then the sample compartment of the pressure vessels is vacuumed. If a microbe sample is included in the sampling programme, the equipment is first sterilised and then vacuumed. So far the PAVE sampler has been used in studies for dissolved gases and microbes.

The salinity of groundwaters at Olkiluoto (TDS_{max} 70 g/l) and Hästholmen (TDS_{max} 35 g/l) increases with increasing depth, suggesting longer residence times and enhanced water-rock interaction. The signs (e.g. high SO₄ and Mg, heavy δ O-18) of the ancient Litorina seawater are most prominent at about 100-400 m. The deep, saline Ca-Na-Cl groundwaters at Olkiluoto have low Eh values, high amounts of S²⁻tot and dissolved gases (mainly CH₄ and H₂) suggesting anaerobic microbiological activity. The deep, saline groundwaters at Hästholmen have much higher amounts of Fe and somewhat lower pH values compared to those at Olkiluoto. The high U contents of the rapakivi bedrock of Hästholmen are reflected in the high He contents of dissolved gases. At both sites the deep (below 500 m), saline groundwaters are mixtures of preglacial meteoric waters and some old, hydrothermal saline fluid. The relative enrichment of Br and Ca compared to Cl and Na in the most saline groundwaters corresponds to the brines from the Canadian and Fennoscandian shields.

1 Introduction

Posiva Oy runs site investigation programmes for final disposal of spent nuclear fuel according to principles laid down by the Finnish Government in 1983. During 1987-92 five sites were studied in preliminary site investigations, also for their hydrogeochemical characteristics (Lampén & Snellman 1993).

Research on three of these sites (Romuvaara at Kuhmo, Kivetty at Äänekoski and Olkiluoto at Eurajoki) continued as detailed site investigations in 1993-1996. The hydrogeochemical characterisation was summarised by Ruotsalainen and Snellman (1996). In 1996 a fourth site, Hästholmen at Loviisa, was included in the site characterisation programme. Hästholmen had been previously studied for disposal of low and intermediate level nuclear waste with several 200 m boreholes also for the hydrogeochemical characteristics (Snellman and Helenius 1992). The final selection of the site will be made in year 2000.

The main objectives of the hydrogeochemical studies are: 1) establishment of a representative data set of groundwater chemistry both horizontally and vertically at each site for hydrogeochemical characterisation before construction of any facilities, 2) evaluation of mean residence times and evolution of deep groundwaters, by geochemical modelling (e.g. Pitkänen et al. 1998; Saksa et al. this proceeding) and 3) acquisition of input data for performance assessment.

After the preliminary site investigations, there was a need to develop the sampling equipment for better reliability and thus development of the PAVE system (Ruotsalainen et al. 1996) was initiated in 1993. The main goals were to sample groundwaters maintaining the in situ-pressure for studies of dissolved gases. The possibility to sterilise the equipment was necessary for representative microbe samples. This paper presents the main ideas of the PAVE sampling system and recent hydrogeo-chemical results from Olkiluoto (Pitkänen et al. 1998) and Hästholmen (Snellman et al. 1998) of groundwater samples taken during 1997. Throughout the paper, "depth" means borehole length, unless otherwise specified.

2 Equipment for groundwater sampling

2.1 PAVE

The name PAVE comes from the Finnish words "<u>paineellisten ve</u>sinäytteiden otin" meaning the equipment for pressurised water samples. All groundwater samples experience a pressure change as they are pumped up to ground level and consequently the dissolved gases will be evacuated. The groundwater samples, collected with PAVE and maintaining the in situ-pressure, give a very good starting point for studying

dissolved gases, microbes, colloids and redox or carbonate sensitive parameters in deep groundwaters.

The PAVE equipment (Figure 2-1) comprises many parts. The wire-line system has one or two inflatable rubber packers to isolate the sampling section from the rest of the borehole (\emptyset 56-76 mm, max. length 1000 m). Above the upper packer there is a combination of 1-3 pressure vessels, 250 ml each. The membrane pump is the uppermost instrument in the borehole. Driven with nitrogen gas and water, the membrane pump lifts groundwater strokewise up to ground level.



Figure 2-1 The PAVE sampler as it is installed in a borehole.

The pressure vessels of the PAVE sampling system are divided into two parts by a movable, o-ring sealed piston. As the pressure compartment of the pressure vessel is filled with argon gas, the piston moves as up as possible in the vessel. Then the sample compartment of the pressure vessels is vacuumed. If a microbe sample is included in the sampling programme, the vessels and all valves with immediate contact with the sample are sterilised and then vacuumed. All these are done before lowering the PAVE sampler to the desired depth into the borehole. The lowering needs a winch and a light rig.

During the pumping period, the chemical quality of groundwater is on-line monitored with electrodes installed in flow-through cells on the ground level as described in section 2.2 and groundwater is by-passing the pressure vessels. In this way microbial bio-films, drilling debris and other fine material will not accumulate on the inner walls of the pressure vessels. When the representativity of the groundwater is good, the sampling for field and laboratory analyses is started. As the final step of the sampling, valves of the pressure vessels are opened increasing hydraulic pressure in the pressure hose for the packers. Then the argon gas in the pressure vessels pressure compartment is compressed, the piston moves downwards, and the sample part is filled with groundwater maintaining the in situ-pressure. Groundwater will be pumped through the pressure vessels for at least some hours, in order to secure a good representativity. Then the valves are closed, the PAVE equipment is lifted to the ground level. The pressure vessels are packed and sent to the analysing laboratories, where Ar gas pressure is coupled to the pressure accumulator side of the pressure vessel. This will move the piston of the pressure vessel upwards and pump a suitable amount of the sample to a prevacuumed separation line and further to analyses (e.g. gas chromatography for dissolved gases).

2.2 Field measurements

Hydrogeochemical field measurements (Ruotsalainen et al. 1998) help to evaluate the representativity of the pumped groundwater and to decide the appropriate time for sampling. Groundwater enters the combination of flow through-cells for measurement of O_2 (one small cell) and Eh, pH, EC and t (a larger cell). The installation box of the flow through-cells is continuously flushed with nitrogen gas to avoid atmospheric contamination. As the down-hole membrane pump works stroke-wise, the measuring system needs an intermediate vessel and a small circulating water pump for maintaining continuous flow. Research and development for more reliable field measurements in very saline groundwaters is under way (Mäntynen 1998).

3 Analytical programmes

Analytical programmes (Table 3-1) have always been adopted according to the character and representativity of the sampling point. When sampling groundwater from deep boreholes, parameters sensitive to atmospheric contamination or transport delay (alkalinity, acidity, Fe^{2+} , Fe_{tot} , S^{2-}_{tot} , anions and NH_4) were analysed in the field laboratory in order to enhance the representativity of the data. These samples have been collected, filtered and, when required, preserved in the N₂ glove box. In addition to samples taken for field and laboratory analyses, a large number of reserve samples preserved in various ways have been taken for possible future use.

Main group	Parameters			
Main variables	pH, EC, density, alkalinity, acidity, DIC			
Anions	HCO ₃ , CO ₃ , Cl, Br, F, I, SO ₄ , S ²⁻ tot, PO ₄ Ntot, Ptot, Btot, Stot			
Cations	Na, Ca, Mg, K, Al, Fe _{tot} , Fe ²⁺ , Mn, SiO ₂ , NH ₄			
Trace elements	Sr, Cs, Li, Ba, Rb, Zr			
Organics	DOC, TOC, uranine (Na-fluorescein)			
Isotopes	δH-2, H-3, δO-18, Rn-222, δC-13(DIC), C-14(DIC) U-234/U-238			
	and U_{tot} (H ₂ O and particles), δ S-34 (SO ₄), δ O-18(SO ₄), δ S-34(S ²⁻),			
	Sr-87/Sr-86, δC-13(CO ₂ , CH ₄), δH-2(CH ₄), δO-18(CO ₂)			
Dissolved gases	N ₂ , O ₂ , CO ₂ , CO, CH ₄ , C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₈ , H ₂ , He, Ar			
Microbes	Total number of cells, Most probable number (MPN),			
	Sulphate reducing bacteria (SRB), Iron reducing bacteria (IRB),			
	Heterotrophic methanogens (HM), Autotrophic acetogens (AA),			
	Heterotrophic acetogens (HA)			

Fable 3	3-1	Analytical	programmes.

Hydrogeochemical studies were all performed according to the field manual for water sampling produced by Posiva Oy (Ruotsalainen et al. 1998). To ensure data quality, control analyses by independent laboratories were carried out for some samples. Special attention was paid to the quality of procedures during sampling, preservation and analysis, using parallel samples and analysis of fresh and/or saline reference groundwaters. Amount of remaining flushing water from drilling activities was controlled by fluorimetric analysis of the tracer, uranine.

4 Results and discussion

4.1 Palaeohydrogeological history of the sites

After the regression of the Weichselian glacier about 10000 BP, both Olkiluoto and Hästholmen remained subaquatic for quite a long time. Olkiluoto rose from the sea around 3000-2500 BP (Eronen & Lehtinen 1996) and Hästholmen about 4000 BP (Anttila 1986). Thus the most saline, post-glacial stage of the Baltic, the Litorina Sea (7500-2500 BP) has effected the local hydrogeochemical conditions at both sites.

4.2 Hydrogeochemical conditions at Olkiluoto

The bedrock of Olkiluoto is mainly composed of migmatitic and veined mica gneisses, quartzitic gneisses, tuffaceous mafic schists, gneissous tonalites or granodiorites and medium grained granites and leucocratic pegmatites (Anttila et al. 1992). The most frequently observed fracture minerals are calcite, iron sulphides (pyrite and pyrrhotite), clay minerals (illite, montmorillonite and kaolinite) and graphite (Gehör et al. 1996). It is noteworthy that no observations of iron oxides or iron hydroxides have been made in the drill core samples. The topography on the Olkiluoto island is very low (max. 18 m) leading to low hydraulic gradients. According to hydrogeological studies (Ahokas et al. 1996), there are more fractures in the uppermost 200 m of the bedrock, and their conductivities are also greater than in deeper parts of the bedrock. Generally, the transmissivities of bedrock structures at the Olkiluoto site range from 10^{-8} to 10^{-4} m²/s (Pöllänen & Rouhiainen 1996).

The hydrogeochemical database of Olkiluoto consists of samples from 11 deep (300-1050 m) boreholes, shallower investigation wells, springs, domestic wells, Baltic seawater, surface waters and precipitation. According to increasing depth, there is a clear zonation of different types of groundwaters in the Olkiluoto bedrock (Pitkänen et al. 1996), Table 4-1.

Depth, m	Salinity	Water type	Origin of dominant end- members	Age estimate, BP
0-150	Fresh- slightly brackish	Na-HCO3	Precipitation Present Baltic seawater	modern - 2500
100-300	Brackish	SO ₄ -rich Na-Cl	Litorina seawater	2500 - 7500
100-500	Brackish	Na-Cl	Pre-Litorina seawater containing fresh glacial meltwater	7500 - 10000
> 500	Saline	Ca-Na-Cl	Preglacial meteoric water, possibly influenced by hydrothermal salts	>> 10000

Table 4-1Main groundwater types at Olkiluoto with origin and age of the
dominant end-members (Pitkänen et al. 1996).

Below the fresh, surface near recent groundwaters, the signs (e.g. high SO₄ and Mg, heavy δ O-18) of the ancient Litorina seawater are most prominent at about 100-400 m. The deep (below 500 m), saline Ca-Na-Cl groundwaters have low Eh values (<-200 mV), high amounts of S²⁻_{tot} (max 3.0 mg/l) and quite high Br/Cl ratios (Figure 4-1) suggesting a hydrothermal origin for the salinity (Pitkänen et al. 1996).



Figure 4-1 Br vs. Cl in the deep, saline groundwaters of Olkiluoto and Hästholmen. Also other data from the Fennoscandian Shield (Pori, Blomqvist et al. 1986, Laxemar, Laaksoharju et al. 1995) is included as reference.

The deep, saline groundwaters at Olkiluoto contain very large amounts of dissolved CH₄ and H₂ suggesting anaerobic microbiological activity (Pitkänen et al. 1996). Before using the PAVE system, dissolved gases collected in glass ampoules on the ground surface hinted to amounts about 30-40 ml/l of CH₄ in the saline groundwaters. The new PAVE samples taken in 1997 have contained as much as 2 litres gas (mostly CH₄) in 1 litre water for the most saline (TDS_{max} 70 g/l) groundwater (Figure 4-2).



Figure 4-2 Dissolved gases in groundwater sample from borehole OL-KR4 (861-866 m).

All of the groundwater samples taken with the PAVE system contained sulphate reducing bacteria (Haveman et al. 1998). Also iron reducers as well as autotrophic and heterotrophic acetogens and methanogens were observed. These results strongly suggest anaerobic conditions for the deep groundwaters at Olkiluoto, in good agreement with the dissolved gas contents.

4.3 Hydrogeochemical conditions at Hästholmen

The island of Hästholmen consists of granitic bedrock located at the western edge of the Wiborg rapakivi massif formed about 1700-1640 Ma ago (e.g. Vorma 1971). Calcite, dolomite, fluorite, iron oxides, iron hydroxides, chlorite and clay minerals (illite, kaolinite, montmorillonite) are common fracture minerals (Gehör et al. 1997a, b). Pyrite occurs only sporadically. Topographically the area is flat (max. 16 m.a.s.l.). According to flow measurement studies (Pöllänen & Rouhiainen 1997) there are some low dipping, highly conductive fracture zones that play an important role in the local hydrogeological conditions.

The hydrogeochemical database of Hästholmen consists of samples from 4 deep (800-1000 m) boreholes, 200 m boreholes drilled in the 1980's, other investigation wells, springs, domestic wells, Baltic seawater, surface waters and precipitation. The main groundwater types (Snellman et al. 1998) at Hästholmen (Table 4-2) are in accordance with those found at Olkiluoto (Pitkänen et al. 1996) reflecting similar palaeohistory. Compared to Olkiluoto, the effects of the ancient Litorina seawaters (high SO₄ and Mg, heavy δ O-18) at Hästholmen seem to be stronger. Also the saline (TDS_{max} 35 g/l) Na-Ca-Cl water below 600 have much higher amounts of Fe and lower pH values. The high Br/Cl ratios (Figure 4-1) refer to a hydrothermal origin for the salinity in the deep groundwaters at Hästholmen, too.

Depth, m	Salinity	Water type	Origin of dominant end- members	Age estimate, BP
0-100	Fresh- brackish	Na-HCO ₃	Precipitation Present Baltic seawater	modern - 4000
100-400	Brackish	SO ₄ -rich Na-(Ca)-Cl	Litorina seawater	4000 - 7500
400-600	Brackish	SO₄-rich Ca-Na-Cl	Pre-Litorina seawater containing fresh glacial meltwater	7500 - 10000
>500-600	Saline	Ca-Na-Cl	Preglacial water, possibly influenced by hydrothermal salts	>> 10000

Table 4-2. Preliminary interpretation of groundwater types, indicative depths and
end-member types for Hästholmen groundwaters (Snellman et al.
1998).

The dissolved gases in the deep groundwaters at Hästholmen seem to have a different composition to those at Olkiluoto. The results strongly suggest reducing conditions with clear observations of CH_4 and H_2 in all analysed samples, but instead of methane, the main gas is nitrogen (Figure 4-3). The content of CO_2 is fairly high possibly reflecting oxidation of organic compounds (e.g. CH_4 to CO_2) during reduction of amorphous iron hydroxides (Snellman et al. 1998). The high amount of He is apparently due to the natural elevated contents of U in the local rapakivi granite.



Figure 4-3 Dissolved gases in groundwater sample from borehole HH-KR2 (850-855 m).

Results from the microbial studies are in good agreement with the general hydrochemical characterisation and the gas results. Iron reducing bacteria were found in all PAVE samples from Hästholmen (Haveman et al. 1998).

5 Conclusions

The recent hydrochemical results from Olkiluoto and Hästholmen, gained with the PAVE system, have greatly improved knowledge on the contents of dissolved gases in deep groundwaters in granitic bedrock. The PAVE sampler has also enabled successful sampling of microbes. Together with other hydrogeochemical data including field and laboratory analyses, the new data of dissolved gases and microbes are in good agreement with the earlier suggested interpretations and further confirm that reducing conditions prevail in deep groundwaters at Olkiluoto and Hästholmen.

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USE OF X-RAY ABSORPTION IMAGING TO EVALUATE THE EFFECTS OF HETEROGENEITY ON MATRIX DIFFUSION

Susan J. Altman, Vincent C. Tidwell, Sean A. McKenna, and Lucy C. Meigs Sandia National Laboratories, Albuquerque, New Mexico, U.S.A.

Abstract

An understanding of matrix diffusion is important in assessing potential nuclear waste repositories in geologic media, as it is a potentially significant process in retarding the transport of contaminant species. Recent work done in evaluating the Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico has brought up two issues that complicate the incorporation of diffusion in Performance Assessment (PA) calculations. First, interpretations of single-well tracer test data suggest that the tracer was diffusing at multiple rates. Second, the estimated relevant rate(s) of diffusion are dependent on the time and length scales of the problem. To match the observed tracer test data, a model with a distribution of diffusion coefficients was required. This has led to the proposal of applying a model with multiple rates of diffusion, the multirate model, to Performance Assessment calculations for the WIPP. A series of laboratory-scale experiments have been designed for the purpose of evaluating heterogeneity and scaling properties of diffusion rates and to test the multirate model.

X-ray absorption imaging was used to visualize and quantify the effects of matrix heterogeneity on the diffusion characteristics for four different centimeter-scale samples of dolomite. The samples were obtained from the Culebra dolomite at the WIPP site. Significant variations in diffusion rates were observed over relatively small length and time (months) scales for the preliminary laboratory experiments. A strong correlation between diffusion rate and porosity was also observed in each of the samples.

Two sets of experiments are planned for 1998. The first set of experiments is similar to those described above. For these experiments, fourteen samples exhibiting a broader range of physical characteristics are being tested. The second set of experiments will visualize the combined effect of advection in a fracture and diffusion into adjacent matrix materials. Tracer solution will flow through an artificial fracture adjacent to a number of blocks of dolomite that have different diffusion rates. This experiment will be used to test the multirate diffusion conceptual model and help parameterize the system.

Our present goals are to improve the understanding of the multirate model and how it can be applied to PA calculations, which are conducted at time and length scales well outside what can experimentally be measured. Our investigations are also being extended to other geological environments. For example, we are currently exploring the extension of these experimental capabilities to the low-porosity crystalline rock such as that located in Äspö, Sweden. This work could be of high value to the TRUE-2 experiment.

1 Introduction

Diffusion is recognized as a potentially important process in the transport of solutes in the subsurface. For example, the *National Research Council* [1994, p.2] identifies diffusion of solutes into "immobile" regions of the subsurface as one of the key technical reasons for the difficulty in predicting and accomplishing aquifer restoration. The transfer of mass via diffusion from high-permeability, advection-dominated domains into and out of low-permeability, diffusion-dominated domains can significantly affect contaminant migration at all scales. Matrix diffusion can also be an important process in providing access to sorption sites within the matrix [*Ball and Roberts*, 1991; *Wood et al.*, 1990]. Understanding and predicting matrix diffusion can, therefore, be critical to environmental remediation programs [*e.g.*, *Wood et al.*, 1990], the recovery of oil [*e.g.*, *Seetharam and Deans*, 1989], and nuclear waste storage in geologic media [*e.g.*, *Neretnieks*, 1980; 1993, *Beauheim et al.*, 1997].

The Waste Isolation Pilot Plant (WIPP) is the U. S. Department of Energy's transuranic waste deep geologic repository in southeastern New Mexico. One of the potential pathways for radionuclides to travel off-site at WIPP is through a fractured dolomite layer located approximately 425 m above the repository. An understanding of matrix diffusion in this unit, the Culebra dolomite, is important to understanding the potential of transport for radionuclides off the site. For this reason, and also to gain a better understanding of diffusion processes, a series of tracer tests were conducted at two locations at the WIPP site [*Meigs and Beauheim*, in preparation]. Interpretations of the tracer tests are presented in *Altman et al.* [in preparation], *Haggerty et al.* [in preparation], *McKenna et al.* [in preparation], *Meigs et al.* [in preparation], and *McKenna et al.* [this issue].

In evaluating the field-scale tracer test data it has been found that multiple rates of diffusion are needed in the model formulation in order to match the single-well tracer test data [*Haggerty et al.*, in preparation]. Furthermore, the relevant rates of diffusion are dependent on the time and length scales of the problem [*Holt*, 1997]. One can consider a system as having a distribution of diffusion rates. The scale (both time and length) of the system controls which diffusion rates are important. At large scales, for example, features contributing to fast diffusion rates may become saturated with solute and no longer contribute to the diffusive response of the system. Also at larger scales, more surface area becomes accessible for diffusion. Close examination of the Culebra shows that porosity exists in many different forms (fractures, vugs, intercrystalline and interparticle) and these different porosity types are present at many different scales [*Holt*, 1997]. These observations provide physical support to the concept of a multirate diffusion model for the Culebra.

The multirate model, previously developed by *Haggerty and Gorelick* [1995], has potential implications for Performance Assessment (PA) calculations. A conventional model of mass transfer with only a single rate coefficient may be an adequate conceptualization only if the time and spatial scale of the experiment being modeled and the total system being assessed are the same. At the laboratory and field scale it may be

possible to determine an adequate integrated single-rate diffusion coefficient. However, such measurements are not possible at the PA scale. To more appropriately perform PA calculations one must address the scaling issues that influence the mass transfer rate coefficients. This can be done by using a distribution of rate coefficients or calculating an integrated single-rate coefficient that accounts for the multiple rates of diffusion that are appropriate at the PA scale [*McKenna et al.*, in preparation].

A series of laboratory-scale experiments have been designed for the purpose of evaluating heterogeneity and scaling properties of diffusion rates. The laboratory-scale experiments provide an opportunity for 1) visualizing diffusion, 2) measuring diffusion rates on different samples, 3) gaining a better understanding of the controls on diffusion, and 4) visualizing advection and diffusion in the same system. The observations and measurements allow us to test the multirate diffusion conceptual model and provide information on the parameterization of the Culebra transport system.

2 Static Diffusion Experiments

2.1 Methods

X-ray absorption imaging is used to visualize and quantify the effects of matrix heterogeneity on diffusion characteristics. Two sets of diffusion experiments have been and are being conducted. The preliminary experiments were run on four, centimeter-scale Culebra rock slabs. Samples were selected so as to capture some of the different porosity types described by [*Holt, 1997*]. Two samples contained vugs (B33-H and RC6-G), one sample contained a large piece of gypsum (RC6-G), one was composed of relatively homogeneous intercrystalline porosity (RC1-A) and the fourth was composed of homogeneous intercrystalline porosity with a fracture running through it (RC2-B). The bulk porosity of the samples ranged from 0.09 to 0.15. These experiments are described and interpreted in more detail in *Tidwell et al.* [in preparation]. A similar set of experiments is currently being run on fourteen samples exhibiting a broader range of physical characteristics of the Culebra.

Samples are set in epoxy on all but one side to approximate no-flow boundaries on these sides. The last side is left exposed to a reservoir. Samples are initially saturated with a background solution of NaCl of equal molar strength as the KI solution used as the tracer. A constant concentration KI boundary condition is achieved by circulating the KI solution through the reservoir at one end of the sample.

X-ray images of the samples are taken at different times throughout the experiment. The transmitted X-ray intensity is a function of the density of the rock at the specific pointed integrated over the full thickness of the slab. Thus, the X-ray intensity is a function of the porosity of the sample as well as the relative tracer concentration at that specific point. The X-ray images are then digitized by placing the film in front of an electronically-controlled bank of high-frequency, high-output fluorescent lights and recording the transmitted light intensity field with a CCD (charged-coupled device) camera. The CCD camera output is digitized into a 1024 by 1024 point array with each point assigned a gray-level between zero and 4095 according to the transmitted light intensity. This resolution results in 0.25-mm by 0.25-mm pixels for these tests.

Using linear absorption theory, the transmitted light intensity through the X-ray can be converted to relative solute concentration (C/C_o) [Tidwell and Glass, 1994]:

$$\left(\frac{C}{C_{o}}\right)_{i,j} = \frac{\ln(I)_{i,j} - \ln(I_{d})_{i,j}}{\ln(I_{s})_{i,j} - \ln(I_{d})_{i,j}}$$
(1)

where C_o is the inlet tracer concentration, I is the transmitted light intensity, I_a is the transmitted light intensity at the same point when it is fully saturated with tracer ($C/C_o = 1$), and I_d is the light intensity at the start of the test ($C/C_o = 0$). Subscripts *i*, *j* refer to the pixel of interest.

Porosity at each pixel $(\phi_{i,j})$ is determined as follows:

$$\phi_{i,j} = \frac{\ln(I_s)_{i,j} - \ln(I_d)_{i,j}}{E[\ln(I_s)_{i,j} - \ln(I_d)_{i,j}]} \phi_{bulk} \frac{z_{i,j}}{z_{avg}}$$
(2)

where $E[\ln(I_s)_{i,j} - \ln(I_d)_{i,j}]$ is the average difference between the tracer saturated and tracerless images, ϕ_{bulk} is the bulk porosity of the rock slab, $z_{i,j}$ is the thickness of the slab at point *i*, *j*, and z_{avg} is the average thickness of the rock slab.

Normalized cumulative mass (M_1/M_1) is calculated along transects parallel to the direction of diffusion as follows:

$$\left(\frac{M_{i}}{M_{\infty}}\right)_{j} = \frac{\sum_{i=1}^{N} \left(\frac{C}{C_{o}}\right)_{i,j} z_{i,j} \phi_{i,j}}{\sum z_{i,j} \phi_{i,j}}$$
(3)

where M_r is the cumulative mass of tracer diffused into the porous medium at time t and M_r is the corresponding quantity when each pixel has reached the concentration C_o , and N is the number of pixels in the transect. The diffusion coefficient can then be calculated from the following equation [Crank, 1975]:

$$D = \frac{0.196l^2}{t_{0.5}} \tag{4}$$

where l is the slab length and $t_{0.5}$ is the time at which $M/M_{2} = 0.5$. Important assumptions made in this solution are that the diffusion coefficient is constant, the porous medium is homogeneous and isotropic, the tracer is conservative, and the boundary conditions are constant throughout the test.

2.2 Results

The first round of diffusion experiments was run for almost 45 days during which time 15 images were generated. Significant variations in diffusion rates were observed over relatively small length and time scales. A more comprehensive discussion of the results and interpretations are presented in *Tidwell et al.* [in preparation].

Figure 1 presents the visual and quantitative data for one sample (RC2-B). This sample has a distinct fracture extending from the inlet boundary to the approximate center of the sample. The fracture is surrounded by a featureless gray dolomite characterized as relatively homogeneous intercrystalline porosity. At early times diffusion is accelerated along the fracture. The front becomes smoother at later times when it has passed the tip of the fracture. Other samples also show a correlation between the spatial distribution of porosity and the diffusion of the KI.

Diffusion coefficients vary by almost an order of magnitude among the four samples and by a factor of 2-3 within the individual samples (Figure 2). The range of measured diffusion coefficients in the second round of experiments is expected to be larger due to the larger variability in the sample characteristics (e.g. samples containing high porosity interparticle dolomite). A larger range of diffusion rates at the field scale is also expected because of the broader range block sizes apparent at this scale.

A strong correlation between diffusion coefficient and porosity is also observed in each of the samples (Figure 3). This plot compares the diffusion coefficients calculated along a transect 1 pixel wide perpendicular to the reservoir face with the corresponding arithmetically averaged porosity. The trend of the correlation between porosity and diffusion coefficient differs for each of the samples. These differences in trend have to do with the differing structures of the heterogeneities. For example, for the sample shown in Figure 1, the porosity of the relatively homogeneous matrix ($\phi = -0.08 - -0.11$) appears to be correlated to the diffusion coefficient. However it can be seen that while the fracture does not have a significant influence on the porosity ($\phi > -0.11$) it does influence the diffusion coefficient significantly. Note that 0.11 is not the porosity of the actual fracture, but an integrated porosity of the fracture and matrix within the pixel containing the fracture.

In contrast to the strong relationship between the pixel scale porosity and diffusion coefficient values, there is not a strong correlation at the bulk sample scale as shown by the large closed symbols in Figure 3. This lack of correlation suggests that diffusion does not simply depend on the magnitude of the porosity but also on how it is spatially distributed. The spatial distribution of the porosity clearly will be related the tortuosity of the sample.

The second round of experiments will be completed in the summer of 1998. To date, porosity measurements have been calculated from these fourteen samples. These porosities ranged from 0.09 to 0.32. These results confirm that there is a large range of porosity values within the Culebra.



Figure 1: Relative concentration fields measured by X-ray absorption imaging showing the diffusion of KI tracer into a brine-saturated slab of Culebra dolomite (sample RC2-B). Also shown is the two-dimensional porosity field. Pictured is a sample characterized by a relatively uniform intercrystalline porosity cut by a single fracture running from the inlet to approximately half the length of the sample.



Figure 2 Diffusion coefficient (equation 4) versus position along the inlet boundary for 4 samples run in the preliminary experiments. The reported diffusion coefficients were calculated for transects one pixel wide.



Figure 3 Scatter plots of porosity versus diffusion coefficient for the four samples run in the preliminary experiments for transects measuring one pixel in width. The four large symbols represent the bulk porosity and diffusion coefficient for the entire rock slab.

3 Advection-Diffusion Experiments

Advection-diffusion experiments are planned to begin in the summer of 1998. The purpose of these experiments is to test the multirate diffusion conceptual model and provide information for scaling from laboratory scale to field scale and ultimately to the PA scale. At present, pre-experimental modeling is being conducted to assist in the design of this experiment.

The experimental set-up will be similar to that described above for the static-diffusion experiments with two exceptions. Instead of one block, several blocks will be lined up in series. The blocks will differ in characteristics based on expected porosities and/or block size (area available for diffusion). As with the static-diffusion experiments, the rock slabs will be potted in epoxy in order to produce no-flow boundaries on all sides except one. On this last side an artificial fracture will be incorporated. A constant flow rate will be run through this fracture, making the advective domain of the experiment.

Theoretically, if two different source terms (*e.g.* different tracer pulse lengths) are used, our controlled multirate system should produce two distinct breakthrough curves. As the pulse length increases, more blocks in the system will become saturated with tracer. As a block becomes saturated, it no longer has an effect on the overall diffusion rate of the system. The block, in essence, "drops out" of the system. Thus with the two pulses, tracer will be diffusing into a different number of blocks at later times in each experiment, thus producing the different breakthrough curves. It is possible that each breakthrough curve or the late time slope of each curve could individually be matched using a single (integrated) diffusion rate. However, this integrated diffusion rate would differ for the two different breakthrough curves using the same diffusion rate distribution.

Through our experimental techniques we will be able to visualize the diffusion through each block and measure the concentrations at the outlet. This information will allow us to determine whether or not diffusion can be visualized at different rates in the different blocks all with the same source term located within an advective front. In addition, through predictive calculations we will be able to test how well we can parameterize the multirate model.

Eventually, we plan to run a visualization experiment on an even more complicated system that begins to approach field conditions. For this setup there will be many layers of blocks of different sizes forming a network of blocks. With this configuration, the advective front will travel on more than one side of each block. This configuration is more analogous to a two-well convergent flow tracer test. With the advective front traveling through a network of blocks we hope to be able to observe under what conditions diffusion is important within a block and under what conditions advection is more important. This test should also contribute to our understanding of the parameterization of the multirate model. This information in turn will contribute to our understanding on upscaling methods.

4 Applications to WIPP and Other Systems

The results of the experiments described above, along with field-testing and numerical modeling work, will be utilized in the design of WIPP PA calculations. This experimental work will contribute the multirate conceptual model, test the parameterization of the multirate model, and assist in the determination of how to apply the multirate model or an appropriate simplified model at different scales (in both time and space).

While the diffusion visualization experiments have been shown to be valuable to a fractured dolomite system, they also have applications to other systems. This technique not only can be used to visualize diffusion, but also has potential for the visualization of other mass-transfer processes, such as sorption. In addition experiments are currently being planned for lower porosity rock types than dolomite. It may be possible to visualize and quantify mass transfer into fractured crystalline rocks, fracture-filling material, and fracture alteration zones.

The multirate mass transfer model also has many applications beyond what is being utilized for the WIPP. In addition to the application to diffusion, there are potential applications to sorptive processes. Causes for the multiple time and spatial scales of sorption in heterogeneous media include variations in the sorptive capacity of the media from variations in mineralogic compositions of the pores to variations in surface area for sorption.

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MATRIX DIFFUSION STUDIES BY ELECTRICAL CONDUCTIVITY METHODS. COMPARISON BETWEEN LABORATORY AND IN-SITU MEASUREMENTS

Yvonne Ohlsson and Ivars Neretnieks Department of Chemical Engineering and Technology Royal Institute of Technology

Abstract

Traditional laboratory diffusion experiments in rock material are time consuming, and quite small samples are generally used. Electrical conductivity measurements, on the other hand, provide a fast means for examining transport properties in rock and allow measurements on larger samples as well. Laboratory measurements using electrical conductivity give results that compare well to those from traditional diffusion experiments.

The measurement of the electrical resistivity in the rock surrounding a borehole is a standard method for the detection of water conducting fractures. If these data could be correlated to matrix diffusion properties, in-situ diffusion data from large areas could be obtained. This would be valuable because it would make it possible to obtain data very early in future investigations of potentially suitable sites for a repository.

This study compares laboratory electrical conductivity measurements with in-situ resistivity measurements from a borehole at Äspö. The laboratory samples consist mainly of Äspö diorite and fine-grained granite and the rock surrounding the borehole of Äspö diorite, Småland granite and fine-grained granite. The comparison shows good agreement between laboratory measurements and in-situ data.

1 Introduction

Matrix diffusion is a process that is of great importance for the retardation of radionuclides escaping from a future repository for nuclear waste. Many laboratory diffusion experiments have been carried out during the last 20 years, and a lot of diffusion data can be found in the literature (Valkiainen (1992), Ohlsson and Neretnieks (1995)). Due to long experimental times it is, however, difficult to use samples that are large enough to represent the intact bedrock. Extensive analysis requirements also limit the number of samples that can be used in a laboratory study. A simple and fast method, both for laboratory and in-situ purposes, would be desirable to make it possible to readily determine the diffusion characteristics of a selected bedrock area. Field measurements would also automatically account for the influence of rock stresses.

For laboratory samples, electrical conductivity measurements have proven a good and fast alternative to traditional diffusion experiments (Skagius (1986)). Larger samples can be used, and the measurements can be used for prediction of the diffusivity of an uncharged species. The latter can be useful for simulation of a "reference species" in diffusion experiments with sorbing species or anions. Due to the negatively charged pore walls, ions are affected by electrostatic forces, and behave differently from uncharged molecules.

Even though large samples can be examined by this method, an in-situ measurement would provide us with matrix diffusion information from measurements under the actual pressure and ground water conditions.

The measurement of the electrical resistivity in the rock surrounding a borehole is a standard method for the detection of water conducting fractures. In this study we intend to evaluate the possibility to use these data for determination of the matrix diffusion characteristics of the bedrock.

2 Theory

Fick's first law applied to a porous medium states that a molecule moves in the

direction of lower concentration under a concentration gradient, $\frac{dC_p}{dx}$:

$$N = -D_{w}\varepsilon \frac{\delta_{D}}{\tau^{2}} \frac{dC_{p}}{dx} = -D_{p}\varepsilon \frac{dC_{p}}{dx} = -D_{w}F_{f} \frac{dC_{p}}{dx}$$
(2-1)

N is the diffusive flux (mole/m²,s), D_w and D_p (m²/s) the molecular diffusion coefficient in the bulk liquid and in the liquid filled pores respectively. ϵ is the dry porosity of the medium, δ_D the constrictivity of the pores and τ^2 the tortuosity. C_p is the pore concentration and F_f is a geometric factor called the formation factor. In the same manner ions will move in an electric field under a potential gradient, $\frac{d\phi}{dx}$ (Atkins 1995):

$$J = -\frac{F}{RT} \sum_{i} z_{i} C_{pi} D_{w,i} \frac{d\phi}{dx}$$
(2-2)

Expressed in terms of electrical conductivity and in a porous medium Eq. (2-2) will have the following appearance:

$$\kappa_{p} = \frac{F^{2}}{RT} F_{f} \sum_{i} C_{p,i} D_{w,i} z_{i}$$
(2-3)

 κ_p is the electrical conductivity due to the ions in the pore solution. In analogy with Eq. (2-1) the formation factor can then be expressed in terms of both diffusivity and electrical conductivity:

$$F_{f} = \frac{D_{p}\varepsilon}{D_{w}} = \frac{\kappa_{p}}{\kappa_{w}}$$
(2-4)

 κ_w is the electrical conductivity due to the ions in the free solution.

The cations that "sorb" only by electrostatic forces to the negatively charged pore surfaces in the rock constitute a swarm of mobile ions in the electrical double layer. Considering this extra transport in the pores results in the following equations for diffusion and for the electrical conductivity respectively:

$$N = -\left(D_{p}\varepsilon + D_{s}\rho K_{d}\right)\frac{dC_{p}}{dx}$$
(2-5)

$$\kappa_{\rm r} = \kappa_{\rm p} + \kappa_{\rm s} = \frac{F^2}{RT} \left(F_{\rm f} \sum_{\rm j} C_{\rm i} D_{\rm w,i} z_{\rm j} + \sum_{\rm j} q_{\rm j} D_{\rm s,j} z_{\rm j} \right)$$
(2-6)

Where D_s is the surface diffusivity and K_d the sorption coefficient (m³/kg). q_j (mole/m³ rock) is the sorbed amount of ion which is described by a sorption isotherm:

$$q_j = K_d C_p \tag{2-7}$$

When the pore water has a low ionic strength, the influence of surface diffusion is large and for highly saline solutions, where κ_w is large, it is insignificant. This is seen in Eq. (2-8):

$$\frac{\kappa_{\rm r}}{\kappa_{\rm w}} = \frac{\kappa_{\rm p} + \kappa_{\rm s}}{\kappa_{\rm w}} = F_{\rm f} + \frac{\kappa_{\rm s}}{\kappa_{\rm w}}$$
(2-8)

3 Methodology and Data

Electrical resistivity data was provided from measurements in borehole KAS02 at the Äspö Hard Rock Laboratory (Data was obtained from the SKB site caracterization database system, SICADA). The rock resistivity was measured in the surrounding rock along the borehole. Also the free ground water resistivity was measured along the hole.

This information has, in this study, been used to evaluate if the in-situ measurements can be used to investigate the matrix diffusion characteristics of the rock and also to evaluate the influence of surface diffusion effects in-situ.

The laboratory samples used in this study are not from KAS02, but they are also from Äspö and the rock composition is similar. The samples mainly consist of Äspö diorite and fine-grained granite while the borehole consists of Äspö diorite, fine-grained granite and Småland granite.

3.1 Laboratory data

The formation factor, F_f , has been determined for laboratory samples by electrical conductivity measurements with highly saline pore water and by diffusion experiments (Ohlsson and Neretnieks (1997), Johansson et al. (1997)). Also the effect of surface diffusion has been studied by electrical conductivity measurements at different ionic strengths (Ohlsson and Neretnieks, 1997). In Figure 2-1 the formation factor for 45 samples with varying length is shown. It is seen that most values lay in a range between $1*10^{-5}$ to $1*10^{-4}$. The spread in results is about the same for the electrical conductivity measurements and the through diffusion experiments, and there is no significant difference between results from the two methods.



Figure 3-1. Formation factors versus sample length for laboratory samples of diorite and fine grained granite from Aspö hard rock laboratory

From electrical conductivity measurements (Ohlsson and Neretnieks (1997)) it has been shown that the relation κ_r/κ_w increases with decreasing ionic strength of the pore solution due to surface conductivity (see Eq. 2-8). For high ionic strength pore solutions the surface conductivity becomes negligible and the value of κ_r/κ_w will be equal to the formation factor. In Figure 3-2 this is shown, and this plot is also used in chapter 4, where laboratory data corrected for variation in ionic strength are used to predict in-situ behaviour.


Figure 3-2. The effect of surface conductivity for different ionic strength pore solutions.

3.2 In-situ data

The electrical resistivity of the surrounding bedrock had been measured by the normal resistivity method (Almén and Zellman (1991)). The measurements are primarily used to locate fractures intersecting the drill hole, and results in a resistivity profile along the hole. Apart from the fractures, the resistivity data also reflects the variation in rock matrix resistivity. To assess the influence of the ionic strength of the pore water on the electrical resistivity of the matrix, the pore water resistivity must also be known

The pore water resistivity data is also provided from the borehole logging. In Figure 3-3 resistivity data has been converted to conductivity (conductivity=resistivity⁻¹), and the rock conductivity as well as the ground water conductivity are plotted along the borehole.

If it were only the pore water conductivity that contributed to the rock conductivity one would expect the rock and the bulk liquid conductivity to follow the same pattern. This is not the case and we will explore if surface conductivity can be a reason for this behaviour.



Figure 3-3 In-situ conductivity data for the rock and the bulk water along the drill hole.

4 Results

From the laboratory results it was seen how the surface diffusion affects the conductivity measurements in different ionic strength pore waters (Ohlsson and Neretnieks (1997)). Using this knowledge and the measured electrical conductivity of the ground water along the drill hole, the in-situ rock conductivity can be predicted along the borehole.

In Figure 4-1 the relation between the electrical resistivity of the pore water to that of the rock, κ_r/κ_w , is plotted along the drill hole. The area within the lines at $1*10^{-5}$ and $1*10^{-4}$ represents the range within which 90 % of the laboratory results are found. Also the ground water conductivity in the borehole is plotted in the same diagram.



Figure 4-1 In-situ conductivity data for the rock and the bulk water along the drill hole.

It can be seen that there is an increase in the ratio, κ_r/κ_w , at around 100-200 m depth compared to values at the deeper parts of the borehole. At 800-900 m depth the high ratio is due to a major fracture zone, which can also be seen from the core description (Stanfors et al. (1997)). Around 100-200 m depth fractures cannot explain the high values of the ratio. Studying the ground water conductivity along the borehole shows that at the depth 100-200 m there is a low conductivity zone. The increased ratio, κ_r/κ_w , at this depth is consistent with the findings from the laboratory experiments and could be due to a contribution from transport of cations in the electrical double layer to the conductivity from the free pore ions.

If the laboratory sample range (the area between the dotted lines in Figure 4-1) is corrected for the variation in ionic strength of the ground water in the borehole, the possibility to predict the appearance of the in-situ plot in Figure 4-1 can be evaluated. This is done in Figure 4-2, where the higher and lower straight lines are corrected for the actual variation in ground water conductivity, which was shown in Figure 3-2. The centre line represents the probable case i.e. the most representative case from the laboratory samples.



Figure 4-2 Prediction of borehole data by correction of laboratory data for changing ground water salinity along the borehole.

In Figure 4-2 correction has also been made for the influence of rock stress on in-situ rock. In laboratory measurements it has been found that the formation factor under stress (300-350 bar) is 20-70 % of the formation factor determined in samples released from stress (Skagius (1986)). Birgersson and Neretnieks (1990) have also showed this in in-situ measurements. A decrease of 50 % was used in this case.

5 Discussion and conclusions

This first attempt to use in-situ electrical resistivity data for comparison with and validation of laboratory results gave promising results. The prediction of the behaviour of the relation κ_r/κ_w from laboratory samples is good

For safety assessment purposes these results lead to interesting possibilities. In-situ electrical resistivity measurements could in the future be used not only to detect fracture zones in an area of interest, but also for determination of in-situ matrix diffusion data. These data are then site specific, and can be used directly in the transport simulation programs used for the safety assessment calculations. Together with knowledge on the nature of the fracture system this would give a direct measure of the suitability of the area as a future repository.

This was a first encouraging test of our hypothesis. The in-situ results from this borehole support the laboratory results, and a continuation will be to look at more borehole data. Especially boreholes with large variations in ground water ionic strength along the borehole would be of interest for further verification of laboratory measurements.

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Session 2b

Modelling

ÄSPÖ MODELLING TASK FORCE – EXPERIENCES OF THE SITE SPECIFIC FLOW AND TRANSPORT MODELLING (IN DETAILED AND SITE SCALE)

Gunnar Gustafson Chalmers University of Technology, Sweden

Anders Ström SKB, Sweden

Peter Wikberg SKB, Sweden

Abstract

The Äspö Task Force on modelling of groundwater flow and transport of solutes was initiated in 1992. The Task Force shall be a forum for the organisations supporting the Äspö Hard Rock Laboratory Project to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock. The group consists of Task Force delegates as well as modelling expertise from eight organisations and meets regularly twice a year. Much emphasis is put on building of confidence in the approaches and methods in use for modelling of groundwater flow and nuclide migration in order to demonstrate their use for performance and safety assessment.

The modelling work within the Task Force is linked to the experiments performed at the Äspö Laboratory. As the first Modelling Task, a large scale pumping and tracer experiment called LPT2 was chosen. This was the final part of the characterisation work for the Äspö site before the construction of the laboratory in 1990. The construction of the Äspö HRL access tunnel caused an even larger hydraulic disturbance on a much larger scale than that caused by the LPT2 pumping test. This was regarded as an interesting test case for the conceptual and numerical models of the Äspö site developed during Task No 1, and was chosen as the third Modelling Task. The aim of Task 3 can be seen from two different perspectives. The Äspö HRL project saw it is a test of their ability to define a conceptual and structural model of the site that can be utilised by independent modelling groups and be transformed to a predictive groundwater flow model. The modelling groups saw it as a means of understanding groundwater flow in a large fractured rock volume and of testing their computational tools. A general conclusion is that Task 3 has served these purposes well.

Non-sorbing tracers tests, made as a part of the TRUE-experiments were chosen as the next predictive modelling task. A preliminary comparison between model predictions made by the Äspö Task Force and the experimental results, shows that most modelling teams predicted breakthrough from all injections, although some teams predicted distinctly lower mass recoveries from those that did not produce a breakthrough. The breakthrough times predicted by the modelling teams are also in accordance with those observed in the experimental results. The evaluation process is on-going.

The STT-1 sorbing tracer test, also part of TRUE-1, was performed in a radially converging flow geometry. The Task No 4E exercise was thus defined with the following overall objectives:

- Develop the understanding of radionuclide migration and retention in fractured rock.
- Evaluate the usefulness and feasibility of different approaches to model radionuclide migration of sorbing species based on existing *in situ* and laboratory data from the TRUE-1 site.

Task No 5 is a hydrological-hydrochemical model assessment exercise which specifically studies the impact of the tunnel construction on the groundwater system at Äspö. The objectives are as follows:

- Assess the consistency of groundwater flow models and hydrochemical mixing-reaction models through integration and comparison of hydraulic and chemical data obtained before and during tunnel construction.
- Develop a procedure for integrating hydrological and hydrochemical information which could be used in the assessment of potential disposal sites.

Introduction

The Äspö Hard Rock Laboratory (Äspö HRL) was constructed as part of the preparations for a deep geological repository of spent nuclear fuel in Sweden. The work within the Äspö Project has been divided into three phases; the pre-investigation, the construction, and the operating phase. The last phase began in 1995. The operating phase is aimed at research and development of models for groundwater flow and radionuclide transport, test of methods for construction and handling of waste and, finally, pilot-tests of important parts of the repository system. The Äspö HRL project co-operates internationally with a number of organisations, all in the field of nuclear waste management. An important part of this co-operation is the work within the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes which was initiated by the Swedish Nuclear Fuel and Waste Management Company (SKB) in 1992.

Each organization supporting the Äspö HRL Project may appoint one qualified specialist as Delegate to the Task Force, see Figure 1.



Figure 1. Illustration of the Äspö Modelling Task Force organization.

Each organization supporting the Äspö HRL is invited to form or appoint a Modelling Team that performs modelling of HRL experiments selected by and/or suggested to the Task Force. Each team may choose to model only a few experiments. The Äspö Hard Rock Laboratory has so far attracted considerable international interest. As of April 1998 eight foreign organizations were participating in the Äspö HRL in addition to SKB. These organizations were: Atomic Energy of Canada Limited (AECL); Power Reactor & Nuclear Fuel Development Corporation (PNC), Japan; Central Research Institute of Electric Power Industry (CRIEPI), Japan; Agence National Pur la Gestion des Dechets Radioactifs (ANDRA), France; Posiva Oy, Finland; Nirex, United Kingdom; Nationale Genossenschaft für die Lagerung von radioaktiver Abfälle (Nagra), Switzerland; and Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie (BMBF), Germany.

Large scale experiments

As the first Modelling Task, a large scale pumping and tracer experiment called LPT2 was chosen. This was the final part of the characterisation work for the Äspö site before the construction of the laboratory in 1990. To be more exact, LPT2 consisted of a three months pumping test combined with a converging tracer test where a number of tracers were injected at different packed-off borehole sections surrounding the pumping borehole. The pumping took place in an open about 600 meters deep borehole and the distance between the pumping and the tracer injection boreholes were in the range 100-300 meters. The entrance points of the tracers into the pumping hole were identified. For the tracer injection sections the groundwater flow through the section was determined by means of a dilution technique. Altogether ten modelling groups using different conceptual and numerical approaches analysed the groundwater flow as well as the tracer experiment outcome, see Table 1. This included deterministic as well as stochastic continuum, discrete fracture network and channel network approaches. The experimental results were available beforehand and this was not a true predictive modelling exercise /Gustafson et al, 1995/.

	Simulation computer code	Continuum/- Discontinuum	Stochastic/ deterministic	Treatment of uncertainties	Density effects
CRIEPI	FEGM/FERM	CONI	DETER	No	No
POSIVA/VTT I	FEFLOW	CONI	DETER ³	- spatial variability of K - sensitivity tests	No ¹
ANDRA/BRGM II	ROCKFLOW	CONT	DETER	No	No ²
ANDRA/BRGM I	MARTHE/SESAME	CONT	DETER	No	Yes
SKB/CFE	PHOENICS/PARTRA CK	CONT	SIOCH ⁴	rock mass conductivity	Yes
PNC/Hazama	SETRA/ARRANG	CONT	STOCH⁴	spatial variability of K	No
NIREX/AEA	NAMMU/NAPSAC	CONT/DISC	STOCH ⁴	spatial variability of K.	No
PNC/Golder	FracMan/MAFIC	DISC	STOCH	FZ hydraulic properties	No
ANDRA/ITASCA	CHANNET/TRIPAR	DISC	DETER	Fracture properties	No ^{1,2}
SKB/KTH	CHAN3D	DISC	STOCH ⁴	spatial variability of K	No
POSIVA/VTT II	**	DISC	DETER	No	No

Table 1.	Modelling	groups	participating	in T	Гask No	1	of the	Äspö	Task	Force	and	selected
model ch	aracteristics	s.						*				

1=density effects considered in separate study

2=salinity varying in space but constant in time Salinity field from MARTHE simulation

3=Stochastic simulations of the flow rate through the tracer injection sections

4=Statistical distributions used for different features in the models, but only one realisation utilised

The construction of the Äspö HRL access tunnel caused an even larger hydraulic disturbance on a much larger scale than that caused by the LPT2 pumping test. This significant hydraulic disturbance was regarded as an interesting test case for the conceptual and numerical models of the Äspö site developed during Task No 1. Hence it was chosen as the third Modelling Task.

The aim of Task 3 can be seen from two different perspectives. The Äspö HRL project saw it as a test of their ability to define a conceptual and structural model of the site that can be utilised by independent modelling groups and be transformed to a predictive groundwater flow model. The modelling groups saw it as a means of understanding groundwater flow in a large fractured rock volume and of testing their computational tools. A general conclusion is that Task 3 has served these purposes well /Gustafson et al, 1997/.

The starting point of each modelling activity was the geologic structural model and its hydraulic interpretation as developed by SKB. However, one of the groups actually chose to study how different structural and conceptual hydrogeological models related to different stages of the Äspö HRL project affected their groundwater flow model results.

In Task 1, the geologic structural model was regarded as robust enough for building a site groundwater flow model. In Task 3, it became evident that important hydraulic connections to the elevator shaft that were needed to explain detailed hydraulic responses were missing. It has been shown that detailed analyses of transient pressure data from the tunnel excavation can provide an improved structural model. However, it is not evident that all the features needed to explain the tunnel and shaft inflows are equally important for the long term geohydrology of the site.

In general, the data deliveries and the formats of these data sets have been of great use for the modellers. However, the data requirements differ depending on the modelling approach used. For example, a modelling approach implementing a discrete feature methodology often needs more raw, non-interpreted, data. By necessity there is a conflicting interest between fast and efficient tunnel and shaft construction, and their characterisation. An example of this was the experience during Task No 3 regarding the data representing the elevator shaft inflow.

The amount of work put into model calibration varies widely among the groups. This is due to the fact that some groups actually did not include this in their objectives. It was found that all types of models could be calibrated to get a reasonable match, except for one borehole. It was also found that calibration gave insight into the features of the site and their connectivity. Successful model calibration is very time consuming and requires a systematic procedure as well as visualisation tools. This is especially true for a large data set like the one available from the tunnel excavation and shaft sinking at Äspö HRL.

A well-developed site conceptual hydrogeological model that includes proper understanding of the boundary conditions is necessary for a successful model calibration. Otherwise, the calibration may result in hydrogeologically unrealistic adjustments of e g the conductivity field. In modelling, an imposed flux boundary condition was preferred for the tunnel and shaft mainly because this avoids the need to define skin effects. On the other hand, this puts more weight on rather uncertain inflow measurements. A no-flow boundary condition on the island of Äspö was considered to be acceptable due to the large impact of the tunnel itself. Using a discrete feature approach, model results indicate that it is necessary to include a permeability decrease at the Baltic sea floor in fracture zones in order to avoid strange boundary effects.

Detailed scale experiments

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

During 1996 a series of tracer experiments in radially converging and dipole flow configurations was performed in a feature using conservative fluorescent tracers and metal complexes. The objectives of the performed tests were specifically to:

- Test transport connectivity
- Test flow heterogeneity
- Determine and compare transport parameters for selected conservative tracers
- Test techniques, tracers and equipment for injection and sampling of tracers in low-transmissive rocks

The TRUE-experiments also consist of sorbing tracer tests. The objectives are to:

- Test equipment and methodology for performing tracer tests with weakly sorbing radioactive tracers
- Increase understanding of transport of tracers subject to sorption in the studied feature
- Obtain parameters which describe retention of tracer transport
- Test different weakly and moderately sorbing radioactive tracers

Task 4 consists of modelling exercises in support of the TRUE tracer tests, see Table 2. Predictive modelling is also performed where the experimental results are not available beforehand.

Modelling Task	Definition/Scope	Status		
4A	To perform modelling in support of the development of a descriptive structural model of the test site	Closed		
4B	To perform modelling in support of experimental design	Closed		
4C	To perform predictive modelling of the radially converging tracer tests in the feature. Comparison of model output with experimental results.	Reporting and evaluation in progress		
4D	To perform predictive modelling of the dipole tests in the feature Comparison of model output with experimental re- sults. Evaluate what can be achieved with existing data set of TRUE-1 in terms of transport predictions for non-sorbing tracers.	Reporting and evaluation in progress		
4E	Performance of predictive modelling of the TRUE-1 tracer tests with sorbing tracers. Comparison of model output with experimental results.	Modelling and reporting in progress		
	Evaluation of what can be achieved with existing <i>in-situ</i> and laboratory data from the TRUE-1 site in terms of predicting transport of solutes subject to sorption.			

Table 2. Modelling Task 4 of the Äspö Task Force group.

For the non-sorbing tracers tests, preliminary comparison between model predictions made by the Äspö Task Force and the experimental results, shows that most modelling teams predicted breakthrough from all injections, although some teams predicted distinctly lower mass recoveries from those that did not produce a breakthrough. The breakthrough times predicted by the modelling teams are also in accordance with those observed in the experimental results. The evaluation process is on-going.

The predictive modelling exercise for the sorbing tracer tests is on-going.

Integration of hydrogeology and hydrochemistry

The groundwater flow and chemistry are important conditions for the safety and performance assessment. In addition to their individual importance these two disciplines would give better confidence in descriptions of the present situation and predictions of future conditions, if properly integrated. The key to a successful integration of the hydrological and hydrochemical models must be to understand the mechanisms behind the processes controlling the evolution and the dynamics of the groundwater system.

An on-going modelling task concerns the impact of the tunnel construction on the groundwater system at Äspö and could be regarded as a hydrological-hydrochemical model assessment exercise. The aim of the task is to compare and ultimately integrate hydrochemistry and hydrogeology. The proposed modelling task will also be useful for a future assessment of the stability of the hydrodynamic and hydrochemical conditions at Äspö. This modelling approach could then be used for any future repository site investigations and evolution, especially in a crystalline bedrock environment.

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 wich could be used for disposal site assessments.
- The basic concept of the modelling task is to utilise the data sets on groundwater chemistry and hydrogeology obtained before and during construction of the Äspö facility.

The modelling task is divided into several sub-tasks where different modelling groups can decide to carry out one or several of them. For the integration of the work two coordinators, one for hydrochemical data and one for geohydrological data, have been appointed.

Summary and conclusions

One important part of safety assessment studies of the disposal systems for spent nuclear fuel is an assessment of the groundwater flow and the effects on radionuclide migration from the repository to the accessible environment. However, predictive modelling of water flow and transport in fractured, low-permeability rock is very complex since the flow is concentrated within fractures. The Äspö Task Force is a forum for the organizations participating in the Äspö Hard Rock Laboratory project to interact in the area of conceptual and numerical modelling of groundwater flow and radionuclide retention in fractured rock.

The modelling exercises on the large scale experiments have provided valuable feedback in understanding site geohydrology by means of an extensive data set representing this large hydraulic disturbance. Furthermore, it demonstrated that model calibration, or corresponding detailed analyses of pressure responses during tunnel excavation, provide an insight into the important hydraulic features of a site. The improvement of a site groundwater flow model by means of using data from long term pumping tests vs. a tunnel drawdown experiment has been discussed. It is evident that the latter provides a much larger data set whereas the former may provide a much more controlled data set. The pumping tests will provide greater confidence in boundary conditions for subsequent modelling. If shafts and tunnels are to be constructed at a site, one should take advantage of this additional large scale hydrological experiment.

The efforts are now turning to the detailed scale and to the tracer experiments part of the TRUE-1 project. The evaluation process of modelling of the non-sorbing tracer tests is on-going. Predicitive modelling of the sorbing tracer tests are taking place at the moment.

Finally, a recently intiated modelling task will focus on the consistency of groundwater flow models and hydrochemical mixing-reaction models through integration and comparison of hydraulic and chemical data obtained before and during tunnel construction. The aim is to develop a procedure for integrating hydrological and hydrochemical information which could be used in the assessment of potential disposal sites.

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Structural conceptual models of water-conducting features at Äspö

Paul Bossart¹⁾, Martin Mazurek²⁾, Jan Hermansson³⁾

¹⁾ Geotechnical Institute Ltd., Berne

²⁾ University of Berne

³⁾ Golder Associates, Stockholm

Abstract

Within the framework of the Fracture Classification and Characterization Project (FCC), water conducting features (WCF) in the Äspö tunnel system and on the surface of Äspö Island are being characterized over a range of scales (centimeters to hundreds of meters). The larger-scale hierarchies of WCF (i.e. features within blocks with sizes >> 10 m) are mostly constituted of fault arrays, i.e. brittle structures that accomodated (often recurrent) episodes of shear strain. The smaller-scale WCF (contained within blocks < 50 m) are single-fracture networks whose mechanistic principles are less straightforward to decipher

The "TRUE-1 block" (corresponding to tunnel meters 2940-3000), i.e. the rock volume in which the first set of crosshole tracer tests of the TRUE project is conducted, has been selected for detailed structural analysis due to the high density of relevant information. In addition to the data obtained from core materials, structural tunnel maps, BIP data and fracture line countings were integrated to derive a structural conceptual model.

The approach to characterise the TRUE-1 block is based on the integration of the following elements:

- Deterministic structural evidence (boreholes, tunnel walls)
- Probabilistic information (fracture statistics, fracture network modelling)
- Down-scaling of observations and concepts derived on a larger scale.

Only a minority of all fractures have lateral extents > 1 m Structural evidence indicates that the fractures within the TRUE-1 block constitute an interconnected system with a pronounced anisotropy.

1 Introduction

The aims of the Fracture Characterisation and Classification Project (FCC) are

- to classify water-conducting features that occur in the Äspö tunnel system
- to characterize and conceptualize 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 characterization of water-conducting features in crystalline rocks.

In the two first phases, the project focused on tectonic discontinuities (transmissive faults) on a scale of meters to tens of meters (MAZUREK et al. 1996). The fault architecture and other relevant properties were studied in the whole Äspö tunnel system as well as on the surface. The ongoing third phase deals with minor discontinuities (scale of decimeters to meters) that occur within blocks delineated by the faults. Much of the work is focussed to the TRUE-1 block, i.e. the rock volume penetrated by the tunnel in the segment 2940 - 3000 m. This site was selected for detailed analysis mainly due to the existence of data derived from cored boreholes and a detailed hydraulic characterisation conducted within the framework of the TRUE project (Winberg, 1996).

The purposes of this paper are to document the status of the FCC project, with an emphasis on the methodology that is being applied to study fractures and faults.

2 Methodology

2.1 Methodology of investigating tectonic discontinuities on the outcrop scale (meters - tens of meters)

The following steps have been applied to derive conceptual models of water-conducting features in faults that discharge water into the tunnel (for details see MAZUREK et al., 1996):

- 1. Preliminary characterisation: A limited number of faults is mapped in detail (lithology, ductile shear-zones, brittle fractures including their trace lengths, orientations, frequencies, fractures infills and wall rock alterations). The aims of this stage are to understand the mechanistic principles of fault development and to derive a catalogue of suitable (site-specific) features and parameters describing the faults.
- 2. Full characterisation: On the basis of the catalogue of attributes, data are acquired from a large number of faults, augmented by hydraulic data (transmissivity, discharge) where available
- Database analysis: A fault classification scheme is developed from the fault database. At Äspö, fault architecture turned out to be the most relevant classification criterion (but other properties, such as embedding host rock, may be more important at other sites).

4. Derivation of conceptual models for radionuclide transport (relevant processes: Advection/dispersion, diffusion, sorption).

2.2 Methodology for conceptualisation of weakly faulted blocks (e.g. TRUE-1)

Given the different scales of observation, the methodology of studying small fractures within a block delineated by faults is different from above and can be divided into three steps (shaded in Figure 2-1).

- 1 **Compilation and update of the database:** The structural database consists of drillcore mapping data, borehole imaging probe (BIP) data and line countings of fractures in the tunnel. The BIP tool provides full-scale images of the borehole walls and allows the derivation of fracture orientations. Line counting includes measuring the frequencies, orientations, trace lengths and other suitable attributes of discontinuities along lines in the tunnels or in surface outcrops. In the tunnel system, information was obtained from lines oriented in three different directions (vertical, parallel to the tunnel axis, horizontal, normal to the tunnel axis).
- 2 Analysis and visualisation of the data: Figure 2-2 visualises and compares fracture patterns derived from drillcore mapping and from BIP imaging along the TRUE-1 boreholes. Fracture frequency derived from core mapping is much higher than that in the BIP data. The core data are affected by artefacts (single-barrel drilling causes artificial fractures), and so the BIP data are considered to represent fracture frequencies and orientations more appropriately. On the other hand, drillcore data are more reliable when the lithologies and the classification of fractures (e.g. mylonites, open fractures, fractures filled with fault gouge) are addressed, and so the two methods were combined for the analysis of the borehole-derived data. Line countings were very useful to derive the trace lengths, especially lines acquired on the tunnel ceiling. The synthesis of these two methods is quite important and leads to the conclusion that ductile precursors (e.g. mylonites) influence the orientation of the fractures and that the fracture network is better interconnected in these areas than elsewhere.
- 3. Derivation of the structural conceptual model: The data selection of steps 1 and 2 results in a fracture network database (including mainly frequencies, trace lengths and orientations). The analysis of fracure orientations shows that 3 sets of fractures can be distinguished (see chapter 3). All these data are compiled in the form of "non Terzaghi corrected" data (contained in the raw database) and "Terzaghi corrected" data. The Terzaghi correction accounts for the smaller probability for fractures running subparallel to the boreholes to be intersected when compared with fractures that are perpendicular to the borehole. The non Terzaghi corrected data can now be used for the derivation of a deterministic model and for fracture network modelling (stochastic part of the structural model), whereas the corrected data are useful for the derivation of generic models.

Methodology: Structural conceptual model of TRUE-1 block



Figure 2-1 Methodology for deriving a structural conceptual model of the TRUE-1 block.



Figure 2-2 Fracture maps derived from a) borehole mapping and b) borehole imaging probe BIP. Projection plane: azimuth 60° , angle of dip 40° , crossing zone of borehole mouths of KXTT1-4.

3 Results

The characterisation and classification of water-conducting features (tectonic faults) on a scale of meters to tens of meters resulted in five structural types that can be reduced into 2 base types (Figure 3-1). Base type 1 consists of a single fault with at least one step per 10 meters along the fault and base type 3 consists of a fault zone. All other types can be derived from overlays of these base types (e.g. type 2 is a swarm of single faults and can be derived by a repetition of single faults). Fracture frequency analyses from the database show that the variability of splay frequencies is much lower compared to that of the master faults. There are preferred orientations of the faults: about 75% of the mapped faults are subvertical and strike NW-SE. Most of the remaining features are steep too but have different strike directions, often SW-NE. Faults could be traced along the tunnel over distances of at least 20 m. Reconnaissance mapping at surface outcrops on Aspö suggests that faults similar to those mapped in the tunnel have extents in the order of tens to hundreds of meters and that along fault strike, the different fault types blend into each other (type 1 may become a type 3 or 5 feature or vice versa). The mineralogy of fracture infills as well as the type of wallrock alteration are identical and cannot be used as distinction criteria for the five fault types.

The geometric parameters of the fracture network of the TRUE-1 block are shown in Figure 3-2. A mean fracture frequency value of 4.5 m^{-1} has been obtained based on the BIP data. Fracture frequencies derived from tunnel-wall maps and line countings are not fully comparable because only fractures >0.2 m in trace length have been considered. There is a clear anisotropy of fracture frequencies, which becomes evident when looking at the stereograms (Figure 3-2). The majority of the fractures contributing to the fracture network are subvertical and strike NW-SE. The dominance of rather short fractures is an important finding for the TRUE-1 block (more than 90 % of the fractures have trace lengths < 1 m). It can be concluded that within the TRUE-1 block, there are only very few fractures with trace lengths larger than one tunnel diameter, and major faults or fault zones seem to be absent. Given the high fracture frequency and the variability of orientation, the fracture network is clearly interconnected.

4 Conceptualisation

A set of conceptual models for larger-scale faults has been derived and presented in MAZUREK et al. (1996). Even in a fault that, on a macroscopic scale, is constituted of one single discontinuity, flow is distributed into a small-scale network of individual fractures that constitute the detailed architecture of the fault. This small-scale flow network can be simplified to orthogonal sets of parallel plates. Fault gouges and cataclasites are located next to the open fractures, and other rock domains close ot the fractures include mylonites, altered rims and fresh rock. In altered host rock porosity is increased, while ductile deformation (mylonites) leads to a reduction of matrix porosity due to recrystallisation. In mylonites, with porosities as low as 0.04 vol%, diffusion is expected to be much less efficient than in rock unaffected by ductile deformation. Fault gouges have enhanced porosities (10-20 vol%) and are well accessible for matrix diffusion (see also Heer and Smith, 1998).



Figure 3-1 Fault geometries of the five types of water conducting features on a scale of meters. $\phi = arithmetic mean$.



Figure 3-2 Frequencies, trace lengths and orientations of fractures in the TRUE-1 block.



Figure 4-1 Generic model of the TRUE-1 block.

At the present stage, the internal structure of the TRUE-1 block (as an example of a block containing mainly small-scale discontinuities) is characterized by a generic and a deterministic model. The generic block model (shwon in Figure 4-1) integrates the fracture geometry on different scales. It starts with a cube of 25 m side length (similar to that of the whole TRUE-1 block) and ends with small cubes of 0.5 m side length. In the latter, the geometries of the lithologies and the fractures are compiled. These parameters show that fracture frequencies in zones affected by ductile deformation (mylonites) are enhanced. Thus the anisotropy of the ductile fabric guides later fracture formation and is responsible for their preferred orientations and increased frequencies. Although an interconnected fracture network exists throughout the TRUE-1 block, zones with ductile precursors represent major flow paths.

The deterministic model combines the geometry of the ductile precursors such as mylonites (from the drillcore database) with the fracture network (from the BIP database). This results in an interconnected fracture network along the boreholes consisting of zones of higher frequencies (mainly bound to the mylonites) which are connected to zones of lower frequencies outwith the mylonites. Correlation of individual fractures inbetween the boreholes is impossible due to the fact that more than 90% of fractures have trace lenghts shorter than 1 m. This leads to two extreme model cases: "highway against network". The highway solution connects the zones with increased fracture frequency but leaves the space inbetween empty. The network solution can be considered as the highway solution plus the filling up of the empty space by stochastic fracture realisations, which obey the results of the fracture geometry (e.g. Figure 3-2). Such realisations are under elaboration at present.

5 Conclusions

- The methodology of characterising and conceptualizing water-conducting features is site-specific and also depends on the scale of observation.
- Small-scale fractures in weakly faulted blocks, such as the TRUE-1 block, can be characterised by data derived from core logging, BIP imaging of the borehole wall, tunnel-wall mapping and line counting.
- Fractures in tectonic faults and fault zones are interconnected with fractures in weakly faulted zones such as the TRUE-1 block.

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EFFECTIVE PROPERTY DETERMINATION FOR INPUT TO A GEOSTATISTICAL MODEL OF REGIONAL GROUNDWATER FLOW: WELLENBERG T⇒K

GW Lanyon GeoScience Ltd, Falmouth Business Park, Falmouth, United Kingdom
P Marschall NAGRA, Hardstrasse 73, Ch-5430 Wettingen, Switzerland
S Vomvoris NAGRA, Hardstrasse 73, Ch-5430 Wettingen, Switzerland
O Jaquet Colenco Power Engineering Ltd, Baden, Switzerland
M Mazurek Rock/Water Interaction Group, Geol. & Min. Pet. Institutes, University of Bern

Abstract

This paper describes the methodology used to estimate effective hydraulic properties for input into a regional geostatistical model of groundwater flow at the Wellenberg site in Switzerland. The methodology uses a geologically-based discrete fracture network model to calculate effective hydraulic properties for 100m blocks along each borehole.

A description of the most transmissive features (Water Conducting Features or WCFs) in each borehole is used to determine local transmissivity distributions which are combined with descriptions of WCF extent, orientation and channelling to create fracture network models. WCF geometry is dependent on the class of WCF. WCF classes are defined for each type of geological structure associated with identified borehole inflows.

Local to each borehole, models are conditioned on the observed transmissivity and occurrence of WCFs. Multiple realisations are calculated for each 100m block over approximately 4000m of borehole. The results from the numerical upscaling are compared with conservative estimates of hydraulic conductivity. Results from unconditioned models are also compared to identify the consequences of conditioning and intervals of boreholes that appear to be atypical.

An inverse method is also described by which realisations of the geostatistical model can be used to condition discrete fracture network models away from the boreholes. The method can be used as a verification of the modelling approach by prediction of data at borehole locations. Applications of the models to estimation of post-closure repository performance, including cavern inflow and seal zone modelling, are illustrated.

1 Introduction

The Wellenberg site in Switzerland has been the subject of detailed geological, geophysical and hydrogeological investigations as the proposed site for the disposal of low and intermediate level radioactive waste. The most recent phase of investigations has now been completed and documented (NAGRA 1997). The aim of the investigations was to derive geological and hydrogeological parameters and understandings for prediction of radio-nuclide transport as part of a safety assessment of the planned repository. The proposed host rock for the repository is the Cretaceous Palfris formation and Tertiary Marls. The Palfris is a highly consolidated argillaceous marl with inter-bedded limestone beds (Mazurek et al. 1998). Figure 1-1 shows a geological cross-section of the site. Seven deep boreholes have been drilled at the site of which five were nominally vertical and two inclined. These boreholes have been the subject of intensive characterisation work including core logging, geophysical logging, hydraulic testing and monitoring.

One of the key hydraulic properties measured in the boreholes is local transmissivity $T(m^2/s)$ of discrete inflow zones. The aim of the work described here is to predict the local scale hydraulic conductivity K (m/s) for input to a geostatistical model of site scale groundwater flow. The methodology for derivation of the conductivities was called "T \Rightarrow K conversion". The T \Rightarrow K calculation method is illustrated in Figure 1-2. The underlying datasets and the steps in the methodology are discussed below.

2 The Hydraulic and Geologic Datasets

As part of the hydraulic testing performed by NAGRA, long intervals of each borehole were isolated and pumped while the borehole fluid was logged using conductivity and temperature probes. It was possible to identify inflow zones from anomalies on the conductivity and temperature logs. Quantitative estimates of inflow transmissivity may also be derived under favourable conditions (Lavanchy & Marschall 1997). Packer testing of isolated intervals was then performed and the results integrated with the fluid logging to derive a final self-consistent dataset. This dataset provided a list of identified zones, estimated transmissivity with uncertainties and detection limits for each borehole. In addition data from the packer tests and borehole monitoring has been used to provide profiles of environmental pressure and groundwater chemistry. During analysis of the packer tests estimates of radius of investigation of each test were made. This was strongly dependent on interval transmissivity and for the majority of the intervals was typically small (<10m) (Lavanchy & Marschall 1997).

Figure 2-1 shows a plot of transmissivity with vertical depth below the top of marl for five of the boreholes. The other two boreholes are close to the margin of the marl and are believed not to be typical of the repository host rock (Jaquet et al. 1997). Only quantified inflow zones are shown on the plot. Other inflow zones have been identified but were of insufficient magnitude to be quantified. There is a clear dependence of transmissivity with depth, with each borehole showing a higher transmissivity interval to about 200m below the top of marl then a transition to much lower transmissivities at

depths of 500m or more. This pattern dominates the observations of feature transmissivity within the host rock and is echoed by the distribution of environmental pressure and groundwater chemistry. The pressures measured within the deeper marks are substantially below hydrostatic. The possible causes of this Under-Pressure Zone are discussed in Vinard et al. (1993).

Although the dominant inflows to the boreholes occur through discrete zones, it was also necessary to determine the properties of the rock between such zones. A small number of packer tests were performed on intervals without inflow zones. The hydraulic conductivities of these tests were between 10^{-12} and 10^{-14} m/s. In addition some tests including inflow features showed conductivities of 10^{-13} m/s or less. The effective hydraulic conductivity of the background rock volume was therefore estimated to be 10^{-13} m/s or lower (Lavanchy & Marschall 1997). It is important to note that this conductivity is probably due to a network of minor discontinuities rather than matrix flow in the strict sense.

Approximately 7 km of core was taken from the deep boreholes. The core was logged for lithology, mineralogy, type and intensity of deformation, fracture frequency, orientation, mineral infill and thickness of highly fractured zones. In addition surface outcrops were mapped to derive information at scales larger than core. Following hydraulic testing and localisation of inflow zones, the core was re-examined in detail at each inflow zone. This detailed examination provided information on one or more potential flow features for each inflow. The information gathered included lithology, degree and style of deformation, porosity and flow wetted surface. A more detailed description of the geological work can be found in Mazurek (1997).

3 T⇒K Conversion Methodology

3.1 Step 1 Evaluation of relationship between geological features and inflow zones

To extrapolate hydraulic properties away from the boreholes it is important to understand the larger-scale geometry of the Water Conducting Features (WCFs).

Key questions regarding the WCFs that needed to be addressed include:

- Which geological types of feature are associated with flow?
- Are geologic properties correlated with flow (e.g. fault orientation, thickness) ?
- How heterogeneous are flow properties within each feature?
- How well connected are the flow areas within each feature and between features?

At a larger scale it is necessary to address the potential influences of lithology, structure, stress and mineralisation on such properties. Within the $T \Rightarrow K$ modelling the dominant depth control on transmissivity (shown in Figure 2-1) was assumed to be typical of the region around each borehole. Other work (NAGRA 1997 and Marschall et al. 1997) has considered the processes that may have caused this depth control.

Integration of core data with the observed inflow zones identified in the boreholes showed that inflow zones were associated with four types of features in the host rock:

- Class 1 Faults (cataclastic zones) in the argillaceous marl
- Class 2 Thin discrete shear zones
- Class 3 Fractured limestone boudins (either isolated or in larger structures)
- Class 4 Joints and other fractures

Class 1 features (faults) were associated with the majority of inflow zones. The fault network at Wellenberg is dense and only a fraction of all faults intersected by the boreholes correlate with inflow zones. In order to understand the hydraulic properties of the host rocks, it is important to understand the basis of this heterogeneity. For example flow might be only associated with faults that had undergone recent reactivation and hence have a particular orientation. Investigation of fault properties showed no correlation between fault orientation, thickness or mineralogy with the hydraulic properties (Mazurek 1997). Thus the observed variability of faults was assumed to relate to heterogeneity within and variability between the faults rather than to separate populations of hydraulically significant faults.

3.2 Step 2 Development of Conceptual Models of the WCF system

For each of the WCF classes a model description was developed from the available information. The level of detail was a function of the importance of the feature class and the information available. The forum for model development was a series of meetings between geologists, hydrogeologists and modellers involved in the project. The data used to parameterise the models were identified and supplemented by expert judgement. In cases where expert judgement was used, ranges of values were suggested.

The most detailed descriptions were developed for the faults (WCF Class 1). Data on all faults greater than 50cm in true thickness had been routinely collected. Data for faults thicker than 10cm had been collected in two boreholes. Orientation data was available for the largest faults and it was assumed that these were typical of the fault population. Length scale was given by a multiplier of the fault thickness (Mazurek et al. 1998). The macroscopic area of each fault was assumed to consist of a) transmissive patches (channels) which relate to the quantified inflow zones; and b) less transmissive (or off-channel) patches that would either be inflows below the limit of detection or intervals with hydraulic conductivity similar to that of the background rock. The channelling fraction (the fraction of channel patches) was calculated from the observed fraction of faults that corresponded to quantified inflow zones in the boreholes. Options for describing the heterogeneity within faults were also considered (see Mazurek et al. 1998).

The transmissivity of the fault channels and of the other hydraulically significant features were described by the transmissivity trend and a local variability derived from the integrated data set. The geometric descriptions of the other WCF classes were simpler than that developed for the faults. A subset of WCF class 3 - the Interbedded Limestone Units were however modelled deterministically throughout the study because

these features might be extensive across the host rock. They are however of low hydraulic significance as the limestone elements are isolated within the structure.

3.3 Step 3 Prediction of Effective Properties

Given a description of the local WCF system around each borehole the effective hydraulic conductivities were calculated for cubes of 100m side-length along the host rock section of each of the five boreholes. Two approaches for the calculation of effective hydraulic conductivity were used (Jaquet et al. 1997).

In the "arithmetic mean approach" the local arithmetic mean transmissivity (over 100m moving window) was divided by 100m (window length) at 50m intervals. This results in an estimate of conductivity similar to that suggested by Snow (1969). It corresponds to the assumption of infinite uniformly transmissive features normal to the borehole. Where features are heterogeneous or of finite size compared to the scale at which the effective properties are required, this approach will be conservative (i.e. over-estimate hydraulic conductivity). However where the transmissive features are steeply inclined to the borehole it is necessary to correct for this orientation bias using a weighting factor (Terzaghi 1965) to determine directional hydraulic conductivity. As only an isotropic conductivity was used in the regional model the arithmetic approach provides a robust procedure that is insensitive to the geological models of WCFs.

The second approach used was the "fracture network approach" where detailed numerical models of the WCF system were constructed for each borehole and the effective conductivity calculated from the numerical models. The NAPSAC discrete fracture network model (Hartley 1998) was used within this study. The fracture network models were conditioned on observed inflow zones and major faults (cataclastic zones) for each borehole. The conditioning method used was based on that described by Chiles (1987) but modified to allow partial conditioning information (e.g. feature type and depth but no orientation). The modified method used a mix of conservative estimates and random sampling of unconditioned models. The random sampling used sample lines of similar orientation to the borehole so that bias was appropriately handled.

The transmissivity of features and patches that did not intersect the borehole, were conditioned using a borehole-specific depth trend. An error function was fitted to the observed \log_{10} transmissivity values. This trend gave the local geometric mean transmissivity of hydraulically significant features (T_{chan}) with depth. The residuals from each fit were assumed to describe the local variability about the trend. The residuals were approximately normally distributed with a typical variance of about 0.5. For each borehole the "unexplained" variance from the error function fit was between 5 and 40% of the total variance in log₁₀ transmissivity.

The NAPSAC calculation of effective hydraulic conductivity was performed for multiple conditioned realisations for both the central case and variants of the WCF models. Mazurek et al. (1998) discuss the effects of different models of the faults. Flows were calculated in three orthogonal directions related to the layout of the regional model. The geometric mean of the three directional conductivities was used to estimate the isotropic hydraulic conductivity. The horizontal axes of the model cubes were aligned with the major strike direction. The boundary conditions used four no-flow boundaries on faces parallel to the flow direction and constant reduced pressure boundaries on the remaining faces. Conductivity tensors could have been calculated (see Hoch et al. 1998), however as an isotropic conductivity was needed, the mean of three directional conductivities was sufficient.

Both the approaches consider only the effective conductivity of the WCF system. In the upper host rock this is the dominant flow system, however where WCF transmissivity is very low (or where WCF frequency declines as suggested by Mazurek et al. 1998) the background rock conductivity may become significant. The host rock effective hydraulic conductivity K_{eff} was assumed to comprise of K_{WCF} and K_{rock} where:

1)
$$K_{eff} = K_{rock} + K_{WCF}$$

Figure 3-1 shows a cross-plot of the arithmetic and fracture network approach derived hydraulic conductivities. Typically the fracture network estimates are one half to one order of magnitude lower than those from the arithmetic mean approach. This is due to the heterogeneity and finite feature size assumed within the fracture network approach. The estimates also show less variability because flow was simulated in a 100m cube rather than being solely dependent on the individual borehole intersections.

Detailed comparison of the two estimates showed that for one borehole the fracture network approach predicted much lower hydraulic conductivities than expected. Further modelling indicated that this was not the case when unconditioned models of this borehole were considered. The effect is due to a particularly low density of the largest faults (>1m thickness). The low density of large faults in this borehole is assumed to relate to heterogeneity of the rock mass.

A question that was also considered at this point was the validity of treating the host rock as an equivalent porous medium on a given length scale. A set of models for transmissivities typical of the repository region was constructed for cube sizes from 50m to 200m side-length. The variation between realisations and cube sizes was small indicating that models were appropriate for the prediction of fluxes at such scales. The relatively small variability between realisations is due to the small variation in transmissivity at the 100m scale. This is due to the removal of the transmissivity trend and to the choice of a single off-channel transmissivity. It is likely that fault transmissivity away from channels varies between just below the detection limit and transmissivities corresponding to the background rock or even the matrix. The models probably therefore over-estimate conductivity but with reduced variability.

The predicted effective conductivities were also evaluated against other evidence from the site. Models of the hydro-mechanical response of the rock mass to glacial unloading suggested that the hydraulic conductivity of the Under Pressure Zone must be very low - at or below those predicted here (Aristorenas and Einstein 1993). Consistency with groundwater chemistry data was considered in another study (Vomvoris et al. 1997).

3.4 Step 4 K⇒T Inverse Model and Verification

The T \Rightarrow K conversion was used as an upscaling procedure for borehole data prior to geostatistical modelling. The geostatistical model (the K Model) of the hydraulic conductivity field for the site (Jaquet et al 1997) used conditional simulation to create multiple realisations. Figure 3-2 shows a cross-section through one realisation, where elements are coloured by log conductivity (m/s). The T \Rightarrow K methodology relied on borehole data to build the detailed WCF system models, so it was necessary to determine an appropriate method for prediction of the WCF system away from the boreholes. Examination of the T \Rightarrow K results suggested a simple relationship between effective conductivity and WCF transmissivity. The relationship is given by equation 2.

2)
$$\log_{10} K_{eff} = lo_{10}T_{Chan} - 2.1$$

where T_{Chan} is the local geometric mean transmissivity (see step 3.3). This relationship together with the dominant transmissivity trend and lack of evidence for major spatial controls on WCF extent or density, allowed the development of the inverse K \Rightarrow T method (Figure 3-3). The K model conductivity field is used to condition WCF system models that assume typical geometric properties. The method was tested by predicting the WCF system around borehole SB3. The predicted transmissivity profile for one realisation is shown in Figure 3-4. The match to the packer test results is good. Packer tests were also simulated using a steady state flow model, the model results were slightly greater than the observed interval transmissivities.

4 Model Applications and Conclusions

The development of the $T \Rightarrow K$ conversion was crucial for up-scaling in a realistic manner that maximised use of geological understanding. It allowed the conversion from discrete points to continuous fields which simplified geostatistical simulation. The methodology also reduced variability by averaging over an appropriate volume and accounting for the effects of borehole sampling.

Having developed the geostatistical models based on the results of the T \Rightarrow K conversion, the K \Rightarrow T method was used to extrapolate the WCF system away from the boreholes. Models of the repository zone were developed for prediction of post closure cavern inflow, transport properties and Excavation Disturbed Zone (EDZ) effects around repository seal zones. Figure 4.1 shows a realisation of the predicted WCF system around the repository zone. The model has been cutaway to show some of the planned repository caverns (shown as red cuboids). Figure 4-2 shows a detail from sample particle tracking calculations performed using the discrete fracture network model around a single cavern.

The integration of geological understanding of the host rock gained from detailed core examination and outcrop mapping with detailed hydraulic characterisation has made it possible to build models of the WCF system that honour the observed WCF properties and are consistent with environmental pressure and groundwater chemistry data. These

models are less over-conservative than previous models where only limited geological input was used to constrain WCF heterogeneity and connectivity.

The development of a combined approach using discrete fracture network models to describe variability at the 10-100m scale with a geostatistical model describing the variability at the site scale, has provided a practical framework for detailed post-closure flow modelling of a heterogeneous host rock. While not addressed in this paper, at the smaller scales required for transport modelling, detailed geological studies of feature porosity and mineralogy have been used to provide appropriate input.

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Figure 1-1 Geological section of the Wellenberg area. Borehole positions are projected onto the plane of the section.





boreholes SB1,SB3,SB4,SB4a/v and SB4a/s





Figure 3-1 Comparison of Arithmetic Mean and Fracture Network Approach derived effective hydraulic conductivity



Figure 3-3 K=>T METHOD: Geometric realisations of the WCF system are conditioned on realisations of the hydraulic conductivity field from K model conditional simulations



Figure 4-1 Predicted WCF system around repository caverns.



Figure 3-2 Section through sample realisation from K-Model conditional simulation using Fracture Network Approach effective conductivities.



Figure 3-4 Predicted inflow transmissivities and packer test measurements for borehole SB3.



Figure 4-2 Cutaway of WCF system around a cavern and sample particle tracks.
ANALYSIS OF TRACER TESTS WITH MULTIRATE DIFFUSION MODELS: RECENT RESULTS AND FUTURE DIRECTIONS WITHIN THE WIPP PROJECT

Sean A. McKenna, Lucy C. Meigs, Susan J. Altman, Sandia National Laboratories, Albuquerque, New Mexico, U.S.A.

Roy Haggerty Oregon State University, Corvallis, Oregon, U.S.A

Abstract

A series of single-well injection-withdrawal (SWIW) and two-well convergent-flow (TWCF) tracer tests were conducted in the Culebra dolomite at the WIPP site in late 1995 and early 1996. Modeling analyses over the past year have focused on reproducing the observed mass-recovery curves and understanding the basic physical processes controlling tracer transport in SWIW and TWCF tests. To date, specific modeling efforts have focused on five SWIW tests and one TWCF pathway at each of two different locations (H-11 and H-19 hydropads).

An inverse parameter-estimation procedure was implemented to model the SWIW and TWCF tests with both traditional and multirate double-porosity formulations. The traditional model assumes a single diffusion rate while the multirate model uses a first-order approximation to model a continuous distribution of diffusion coefficients. Conceptually, the multirate model represents variable matrix block sizes within the Culebra as observed in geologic investigations and also variability in diffusion rates within the matrix blocks as observed with X-ray imaging in the laboratory. Single-rate double-porosity models cannot provide an adequate match to the SWIW data. Multirate double-porosity models provide excellent fits to all five SWIW mass-recovery curves. Models of the TWCF tests show that, at one location, the tracer test can be modeled with both single-rate and multirate double-porosity models. At the other location, only the multi-rate double-porosity model is capable of explaining the test results.

Introduction

A number of single-well injection-withdrawal (SWIW) and two-well convergent flow (TWCF) tracer tests have been conducted in the Culebra Dolomite member of the Rustler Formation in the vicinity of the Waste Isolation Pilot Plant (WIPP) in southeastern New Mexico. These tracer tests were conducted with the goal of better characterizing the physical transport parameters of the Culebra dolomite and the test results are summarized in Meigs and Beauheim [in prep].

The Culebra Dolomite is roughly 7 meters thick in the area of the WIPP site. The Culebra represents a potential pathway for off-site migration of radionuclides under the scenario of human intrusion into the repository. The Culebra is well fractured and, for the modeling results presented herein, the hydraulic conductivity can be considered as an effective continuum. The transport properties of the Culebra are conceptualized as a double-porosity system with advection through the connected fractures and solute storage occurring in the matrix blocks and in dead-end fractures.

The goal of this paper is to elucidate the processes responsible for mass transfer in the Culebra Dolomite. Toward this goal, we are interested in developing a model of mass transfer between fracture and matrix porosity, or more generally between advective porosity and diffusive porosity, and testing that model on data acquired in a number of SWIW and TWCF tracer tests.

1.1 Mathematical Model

The multirate model [*Haggerty and Gorelick*, 1998] enables mass transfer to be modeled with a continuous distribution of diffusion rate coefficients. Variability in matrix block sizes and tortuosity can cause a distribution of diffusion rate coefficients. For sorption processes, mass transfer is viewed as a first-order surface reaction. The surfaces involved may be those accessed by advection, diffusion or some combination of these transport processes. Total mass transfer within an aquifer can be any combination or probability density function of diffusion or surface reaction processes [*Haggerty and Gorelick*, 1995].

In this paper, we are concerned solely with diffusion processes and interpretation of tracer tests done with non-sorbing tracers (benzoic acids). The multirate mass transfer model presented here is similar to that described by *Cunningham et al.* [1997] and *Haggerty and Gorelick* [1998]. Diffusion is assumed to occur along one-dimensional pathways within the matrix blocks, and it is assumed that mass-transfer properties are homogeneous along each pathway and that the pathways are independent of one another. The pathways and matrix blocks can be any shape as long as the diffusion rate coefficients form a continuous distribution. In this work, we employ a log-normal distribution of diffusion rate coefficients for reasons discussed in *Haggerty and Gorelick* [1998].

The equations for solute transport into or out of a well, in the presence of a lognormal distribution of matrix diffusion processes, is given by (after *Haggerty et al.* [in press]):

$$\frac{\partial c_a}{\partial t} + \int_0^\infty \beta(\alpha_d) \frac{\partial c_d(\alpha_d)}{\partial t} d\alpha_d = \frac{1}{r} \frac{\partial}{\partial r} \left(\frac{r\alpha_L |\nu|}{R_a} \frac{\partial c_a}{\partial r} \right) - \frac{\nu}{R_a} \frac{\partial c_a}{\partial r}$$
(1)

$$\beta(\alpha_d) = \frac{\beta_{tot}}{\sqrt{2\pi}\sigma_d \alpha_d} \exp\left\{-\frac{\left[\ln\left((\alpha_d) - \mu_d\right)\right]^2}{2\sigma_d^2}\right\}$$
(2)

where:

$$\alpha_d = \frac{D_a}{l^2} \tag{2b}$$

and

$$\beta_{tot} = \frac{\phi_d R_d}{\phi_a R_a} \tag{2c}$$

and where c_{α} [M/L³] is the solute concentration in the advective porosity (e.g. fractures); \overline{c}_d [M/L³] is the average solute concentration in the portion of the matrix associated with a particular diffusion rate coefficient; α_d [1/T] is the diffusion rate coefficient described in (2b), which is continuously distributed; $\beta(\alpha_d)$ [-] is the capacity coefficient as a function of the diffusion rate coefficient probability density function (PDF). We assume the diffusion rate coefficient PDF to be lognormal in (2a); β_{tot} [-] is the total capacity coefficient of the formation, which is the ratio of mass in the matrix to mass in the fractures at equilibrium; v [L/T] is the pore-water velocity; R_a [-] is the retardation factor in the advective porosity; r [L] is the radial coordinate (positive away from well); t [T] is time elapsed since the beginning of injection of the first tracer; σ_d is the standard deviation of the log-transformed diffusion rate coefficients; md is the natural log of the geometric mean of the diffusion rate coefficients; D_a [L²/T] is the apparent diffusion coefficient in the matrix, which may be defined most simply as the product of the aqueous diffusion coefficient of the tracer and diffusive tortuosity, although this expression may be modified to incorporate processes such as immobile zone sorption; l [L] is the length of the diffusion pathway within the matrix; ϕ_d [-] is the diffusive porosity of the formation; and R_d is the retardation factor due to sorption within the diffusive porosity; ϕ_a [-] is the advective porosity. Equations describing the concentration distribution within the diffusive porosity along with boundary conditions for the solution of these equations in SWIW and TWCF systems are discussed in *Haggerty et al.* [in prep] and *McKenna et* al., [in prep].

Detailed examination of geology in many subsurface environments suggests that a distribution of mass-transfer rates arising from variation in block sizes is geologically more plausible than the single matrix block size ("sugar cube") conceptualization employed in standard double porosity models (Figure 1). Equation 2 not only defines this distribution of diffusion rate coefficients, assumed to be lognormal in this work, but provides a critical link between the diffusion rate coefficients and the solute storage capacity of the diffusive porosity associated with each rate coefficient. Equation 2 ties each diffusion rate coefficient, α_d , to a specific volume of storage. This volume is specified as a fraction of the total storage capacity of the medium, β_{tot} , and is expressed as a function of the diffusion rate coefficient $\beta(\alpha_d)$. At equilibrium conditions, $\beta_{tot} = \phi_d / \phi_{a^{-1}}$ Also, it is noted that in (2b) variability in α_d is due to variability in both *l* and τ and that the joint variability cannot be further refined.

1.2 Damkohler Number

For a given experimental setup and duration, the diffusive impacts of only a limited range of block sizes can be investigated directly. The ability of the multirate model to estimate the diffusion rate coefficient distribution is limited by the ratio of diffusive to advective mass-transfer rates within the tracer test system. The ratio of diffusive to advective mass transfer can be parameterized with the (dimesnionless) type I Damkohler number, *DaI*. For a one-dimensional flow system with first-order diffusive mass transfer into layers, the type 1 Damkohler number is [after, *Haggerty and Gorelick*, 1995]:

$$DaI = 3\alpha_d(\beta(\alpha_d) + 1)\frac{RL}{\bar{\nu}}$$
(3)

where L [L] is the transport length and $\overline{\nu}$ [L/T] is the average velocity along the transport path. Damkohler numbers near 1 indicate that the rate of diffusion is similar to the rate of advection. At a Damkohler number of 100 or larger, diffusion can be considered instantaneous relative to advection and the local equilibrium assumption (LEA) applies [Bahr and Rubin, 1987]. In this situation, the porosity available for solute transport is equal to ($\phi_a + \phi_d$). Conversely, at a Damkohler number of 0.01 or smaller, diffusion is negligible relative to advection at the time and geometric scales of interest, and a single porosity (ϕ_a) numerical implementation of the overall conceptual model for transport will be adequate.

The Damkohler number can be examined across the distribution of mass-transfer rates in a radial flow system by considering the average velocity along a flowpath from an arbitrary starting radius, R_o , to the extraction well radius, $r_w (L = R_o - r_w)$. We apply the Damkohler number limits to the TWCF test data to determine the resolution of the tests in terms of defining diffusion rate coefficients.

Simulation of Tracer Test Data

Five SWIW and two pumping-injection well pairs are analyzed. Both types of tests were conducted at the H-11 and H-19 hydropads near the WIPP site. The different benzoic acid tracer tests will be referred to by the hydropad. All fluid and tracer injection and withdrawals were done across the full aquifer thickness. Further details regarding the physical setup and data collection of the tracer tests can be found in *Meigs and Beauheim* [in prep].

The SWIW tests were accomplished by injecting a tracer and a Culebra-brine chaser into the Culebra. After a rest period of approximately 17 hours, the well was pumped and the discharge was sampled for up to 1000 hours to determine the mass recovery curve. Two TWCF tests are considered here. The H-11 test was run at a constant pumping rate for approximately 25 days after injection of the tracer. During this time period, 107 samples were collected and analyzed for concentration. For the H-19 tracer test, 67 samples were collected during a pumping period of 29 days.

Parameter estimation applied to the multirate diffusion model discussed above is used to provide an optimal fit of the model to the observed data. The parameter estimation minimizes the root mean square error (RMSE) between the log of the observed data and the log of the predicted concentration. Four parameters are estimated: the mean ln diffusion rate coefficient, μ_d , the standard deviation of the ln diffusion rate coefficient distribution, σ_d , the advective porosity, ϕ_a , and the longitudinal dispersivity, α_l . The parametric expression of diffusion rate coefficients used here is a log-normal distribution which is fully characterized by its mean and standard deviation. The estimated parameter values and the RMSE statistic obtained with the multirate model are given for the H-11 and H-19 tests in Table 1. Modeled results are shown with the observed data in Figures 2A and 2B for the H-11 and H-19 SWIW tests and in Figure 3 for the H-11 and H-19 TWCF tests.

Results shown in Figures 2 and 3 are based on estimated log-normal distributions of diffusion coefficients. The cumulative matrix volumes as a function of diffusion rate coefficient as determined from the inverse parameter estimation using the multirate model are shown in Figures 4A and 4B for both the SWIW and TWCF tests. Examination of Figure 4 shows that there is a large difference in the distributions between the H-11 and H-19 hydropads. For both types of tests, the standard deviation of the diffusion coefficient distribution is much larger at H-19 than at H-11.

2.2 Resolution of Tracer Tests

The portion of the log-normal distributions that can actually be resolved during the tests is determined by applying the Damkohler number limits of 0.01 and 100. The changing flow velocities and rest period of the SWIW test make calculation of the Damkohler limits quite complex. Here we use a conservative approximation of those limits as described in Haggerty et al [in prep.]. As shown in Figure 4A, the SWIW tests show that roughly 80 percent of the diffusion rate coefficient distribution lies within the Damkohler limits at the H-11 hydropad. For the H-19 SWIW tests, approximately 70-80 percent of the distribution lies within the limits.

For the TWCF tests, the H-11 hydropad has roughly 85 percent of the diffusion rate distribution within the 0.01 and 100 Damkohler number limits, while at the H-19 hydropad approximately 55 percent of the distribution lies within the limits (Figure 4B). Consequently, at the H-19 hydropad approximately 30 percent of the estimated diffusion rates are so small as to be negligible and approximately 15 percent of the rates are fast enough to appear instantaneous. The distribution of diffusion coefficients is effectively inestimable outside these Damkohler limits and only has shape in those regions because of the *a priori* assumption of a log-normal distribution.

The consistency of the estimated, log-normal distributions of mass-transfer rates can be checked by determining the estimated matrix block size distribution. All variability in the mass transfer rates can be assigned to variations in matrix block size by assuming a constant tortuosity and then comparing estimated matrix block lengths to field observations. For one-dimensional diffusion paths into the matrix, it is possible to calculate the distance from the fracture/matrix interface to the center of the matrix block, 1, (matrix block 1/2 length) by rearranging equation (2b). Using measured values of aqueous diffusion coefficient, D_o , and average values of τ as measured in core samples (0.09 at H-11)

and 0.11 at H-19), solution of equation (2b) shows that the SWIW are capable of resolving block sizes from $< 2x10^{-04}$ meters to 0.20 meters. The TWCF tests were able to resolve, within the Damkohler limits, a range of half-block sizes from < 0.001 to 0.13 meters at the H-11 hydropad and from 0.002 to 0.13 meters at the H-19 hydropad. These estimates of block size are consistent with the lower end of the range of block sizes observed in core and outcrop samples [*Holt*, 1997].

Previous to this work, only single-valued diffusion rates have been applied to the analysis of two-well, double porosity tracer tests. To compare the results of the multirate model to the traditional, single-rate (double porosity) approach, single-rate model runs were completed using parameter estimation for the tracer tests at each hydropad. This estimation procedure is the same as that used for the multirate model; however, σ_d is set to 0.0. In order to maintain consistency, these single-rate runs were constrained to have the same total porosity ($\phi_a + \phi_d$) as derived from the multirate modeling. Results of the single-rate matches to the observed data are given in Table 2 and Figures 5A and 5B. Note that single-rate solutions could only be obtained for two of the five SWIW tests.

In general, the single-rate of mass transfer is smaller (larger negative number) than the mean of the multirate distribution for both of the TWCF tests modeled. The estimated mass-transfer rate using the traditional double-porosity model results in matrix halfblock sizes of 0.11 and 0.03 meters in the SWTW tests and 0.18 and 0.33 meters at the H-11 and H-19 hydropads respectively. Additionally, the advective porosity estimated with a single-rate model is higher than that estimated with the multirate model. For the H-19 TWCF test, this increase in ϕ_a is over an order of magnitude (Table 2). As measured by the RMSE, the multirate model provides a significantly better fit to the data than does the single-rate model for all tests with the exception of the H-19 TWCF test. The RMSE of the single-rate model fit for the H-19 TWCF test is only slightly higher than that obtained with the multirate model.

Conclusions

The multirate diffusion model developed previously for one-dimensional flow [Haggerty and Gorelick, 1995] is extended to the case of a convergent flow system with a injection at radial distance from the pumping well. This model has been applied to the results of the H-11 and H-19 tracer tests conducted in the Culebra dolomite at the WIPP site. Model results show significant differences in the diffusion process at the two hydropads. At the H-11 hydropad, the multirate diffusion model is necessary to describe the break-through curve.

Models developed with data from a SWIW test are not necessarily transferable to a TWCF test. The fast end of the diffusion rate distribution is better estimated with a SWIW test because of the insensitivity of that test to advective porosity. The portion of advective porosity that is due to instantaneous diffusion rates or in fact is actually fracture porosity, may be indeterminate in a TWCF test. At H-19, the insensitivity of the SWIW test to advective porosity made it impossible to model that test with a single-rate model. However, it is possible to model the H-19 TWCF with an increased advective porosity to account for the instantaneous diffusion and fit the data with a single-rate model.

In the TWCF tests at the H-19 hydropad, the choice of a conceptual model (multirate over single-rate) is non-unique. Both models did an adequate job of fitting the TWCF test. Calculation of Damkohler numbers across the distribution of diffusion coefficients shows that roughly 50 percent of the estimated distribution is beyond the resolution of the tracer test and thus cannot be estimated with any confidence. The single-rate model can be viewed as a multirate model with two discrete mass-transfer rates: instantaneous and extremely slow. The instantaneous rates are modeled in a single-rate model as advective porosity and the single-rate is estimated to be very slow (infinite block size). More work is necessary to determine if multi-modal or other non-parametric distributions can be used to model the tracer breakthrough curves at H-19.

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Test	Estimated Parameters						
SWIW	Ф _{аdv}	α_l	μ _d	σ _d	RMSE		
H11-1	1.6x10-03	0.06	-16.5	3.6	0.18		
H11-2	4.7x10-03	0.07	-16.0	3.8	0.26		
H19S2	1.1x10-02	0.18	-10.6	5.7	0.15		
H19S1-1	4.9x10-03	0.21	-11.9	6.9	0.08		
H19S1-2	2.1x01-02	0.12	-10.1	2.64	0.17		
TWCF							
H-11(L)	8.1x10-04	3.4	-17.6	1.3	0.10		
H-19(L)	3.8x01-03	1.0	-16.2	5.5	0.11		

Table1: Parameters estimated with the multirate model on SWIW and TWCF tests.

Table 2: Parameters estimated with the single-rate model on SWIW and TWCF tests. It was not possible to fit three of the SWIW tests with a single-rate model.

Test	Estimated Parameters					
SWIW	ф _{аdv}	α_l	μ _d	σ _d	RMSE	
H11-1	7.1x10-03	0.46	-18.8	0.0	0.51	
H19S1-1	5.4x10-02	0.16	-16.2	0.0	1.21	
TWCF						
H-11(L)	1.5x10-03	0.9	-19.8	0.0	1.83	
H-19(L)	5.7x10-02	2.4	-21.1	0.0	0.16	



Figure 1. Conceptual model for multirate diffusion.



Figure 2. SWIW data and multirate model fits to the data for A) H-11 and B) H-19.



Figure 3. TWCF data and multirate model fits to the data for H-11 and H-19.



Figure 4. Cumulative distributions of diffusion rate coefficients as determined with the multirate model for the (A) SWIW tests and (B) TWCF tests. The Damkohler limits are defined by the vertical dotted lines in (A) and the bold portion of the lines in (B).



Figure 5. Single-rate model fits to the (A) SWIW tests and (B) the TWCF tests. Note that single-rate models could only be obtained for two of the SWIW tests.

FIELD APPLICATIONS OF THE CHANNEL NETWORK MODEL, CHAN3D.

Behrooz Khademi, Björn Gylling, Luis Moreno and Ivars Neretnieks Department of Chemical Engineering and Technology, Royal Institute of Technology. Kemakta Konsult AB, Box 12655, S-112 93 Stockholm, Sweden.

Abstract

The Channel Network model and its computer implementation, CHAN3D, was developed to simulate fluid flow and transport of solutes in fractured media. The model has been be used to interpret field experiments of flow and transport in small and in large scale. It may also be used for safety assessments of repositories for nuclear and other hazardous wastes. In this case, CHAN3D has been coupled to a compartment model, NUCTRAN, to describe the near field of the repository.

The model is based on field observations, which indicate that the flow and solute transport take place in a three-dimensional network of connected channels. The channels have very different properties and they are generated in the model from observed stochastic distributions. This allows us to represent the large heterogeneity of the flow distribution commonly observed in fractured media. Solute transport is modelled considering advection and rock interactions such as matrix diffusion and sorption within the interior of the rock. Objects such as fracture zones, tunnels and release sources can be incorporated in the model.

The most important site-specific data for the Channel Network model are the conductance distribution of the channels (mean value and standard deviation) and the flow-wetted surface. The latter is the surface area of the rock in contact with the flowing water. The relationship between the flow-wetted surface and the water flow is a crucial entity for radionuclide transport. The conductance distribution of the channels and the flow-wetted surface may be estimated from hydraulic measurements. For the Äspö site, several borehole data sets are available, where a packer distance of 3 metres was used. These boreholes data have been studied in detail to determine transmissivity distributions and correlation length for each of the boreholes.

In order to study uncertainties in the determination of the flow wetted surface and conductance distribution some numerical experiments were performed. Synthetic data were generated along a borehole and hydraulic tests with different packer distances were carried out. In each borehole a given number of fractures are randomly located.

1 Introduction

Deep repositories in crystalline rocks are a possible solution to the disposal of hazardous waste, including nuclear waste. The performance assessment of these repositories requires use of models that calculate the transport of contaminants to the biosphere. Fluid flow and solute transport in fractured rock are poorly described by the advection-dispersion concepts and equations. Moreover, field observations show that there are strong channelling effects and that when attempts are made to evaluate the dispersion coefficient, it appears to increase with distance.

Fluid flow and solute transport in fractured rock occur mainly through fractures and fracture zones. Due to the heterogeneities on the fracture surfaces the fluid flow occurs mainly through preferential paths where solutes are transported by the flowing water. Solutes may migrate into the stagnant water in the rock matrix surrounding the channels. Sorbing solutes may also be sorbed on the micropore surfaces. These two mechanisms may significantly retard the transport of solutes in fractured media. On the other hand the existence of these preferential paths, channelling, may cause solutes in such paths to travel considerably faster than the average velocity.

Based on the fact that fluid flow and solute transport in fractured media occurs through a network of individual channels, the Channel Network model was developed (Moreno et al., (1993)). The model has been used to carry out a performance assessment of a repository for final disposal of radioactive waste (Gylling et al., (1997b)). This model has previously been applied to the study of water flow in the SCV Stripa experiment (Birgersson et al., (1992)) and to study the Longterm Pumping and Tracer test (LPT2) carried out in the Hard Rock Laboratory (HRL) at the island of Äspö (Gylling et al., 1997a). Recently, the model has been used to simulate the TRUE experiment at HRL (Gylling et al. (1998)). Application of the Channel Network model to the tracer tests with sorbing solutes in the TRUE experiment is shown in this paper.

In the paper, it is also shown how the conductance distribution of the channels and the flow-wetted surface may be estimated from hydraulic measurements. In order to address the importance of the packer distances used in the hydraulic tests, some numerical experiments were performed. These numerical tests were also used to estimate the volume of data needed to obtain a reliable value for this parameter. These are very important issues to be addressed since data gathering is very costly.

Data of several boreholes from the Äspö site, obtained by using a packer distance of 3 m, are available. They were used to characterise the hydraulic data from the site. Mean hydraulic conductivity (geometrical mean) and the correlation structure were determined from these data. They were also used to compare some of the results from the numerical tests.

The aim of this paper is twofold. Firstly, to show how the Channel Network model may be applied to a specific site. Secondly, to address the importance of the packer distance used in the hydraulic tests.

2 The Channel Network Model

In the channel network model it is assumed that the flow paths make up a channel network in the rock. Every channel can connect to any number of other channels, but we choose an upper limit of six channels intersecting at a point. The use of six channels is partially based on the observation that both fracture intersection and channels in the fracture plane play an important role in conducting flow. This is illustrated in Figure 2-1. Some of these channels may have a conductivity that is so low that no connection is made.

In the model concept, fluid flow and solute transport take place in a network of channels, for visualisation purposes, the network is depicted as a rectangular grid. Data can be obtained from borehole transmissivity measurements and observations on fracture widths in drifts and tunnels. Flow calculations need only the information on the conductance of the channel members and the boundary conditions. The conductance is defined as the flow rate in a channel member divided by the pressure difference between its ends. When solute transport for non-sorbing species is included, the volume of the channels has to be known. If sorption onto the fracture surface or diffusion into the matrix is included in the model, the area of the flow-wetted surface must also be known. Some properties of the rock are also needed, such as rock matrix porosity, diffusivity and sorption.



Figure 2-1 A schematic view of the model concept.

In the present simulations, it is assumed that the conductances of the channel is lognormally distributed and not correlated in space. Once that the fluid flow is calculated, the solute transport is simulated by using a particle-following technique (Robinson (1988), Moreno et al. (1988)). Many particles are introduced, one at a time, into the known flow field at one or more locations. The residence time of an individual particle is the sum of residence times in every channel that the particle has traversed. The channel volume is estimated by assuming that the conductance of the channels is proportional to the cubed channel aperture, owing to the lack of data. Hydrodynamic dispersion in the channels is considered to be negligible.

3 Data needed by CHAN3D

In order to assess the flow distribution in the network, CHAN3D needs data on the conductance distribution of the channels. For nuclides, which interact with the rock matrix, the flow-wetted surface is an essential entity in transport calculations, in addition to diffusion and sorption properties of the rock matrix.

The mean conductivity of the rock mass may be estimated from borehole data. For the channels in a given fracture zone, the mean conductance is calculated from the transmissivity of the fracture zone. The standard deviation of the channel conductance is also estimated from these borehole data. There is no need to determine any dispersivity as the model structure inherently generates the spreading effects otherwise attributed to "dispersion".

To obtain the flow wetted surface area, consider a rock volume with a number of channels randomly distributed in the space which have an average length L, and a average width W. A borehole drilled through this rock mass will intersect, on average, a channel each H m. Now, the number of channels in a given rock volume has to be correlated to the frequency that channels are intersected by a borehole. To do this, the average projected area of the randomly located channels is redistributed over a plane with a separation between them equal to the borehole diameter. Thus, the average area A_{av} needed for a channel to be intersected by a borehole is

 $A_{av} = A_{proj} + (W_{proj} + L_{proj}) D_{bh} + D^2_{bh}$. This area includes the projection of the channel area and the space occupied by the borehole itself. Since the channels can be randomly oriented in space, the mean value of the projected lengths and widths of the channels in a plane are $L_{proj} = (\pi/4) \cdot L$ and $W_{proj} = (\pi/4) \cdot W$ respectively. If the average distance between channels intersected by the borehole has been obtained as H, then the average rock volume containing one channel is HA_{av} . The specific flow-wetted surface, a_R , is the surface of the channel, 2A, in the rock volume HA_{av} . Thus:

$$a_{R} = \frac{2 \cdot A}{H\left[\frac{A}{2} + \frac{\pi}{4} \cdot D_{bh}(W + L)\right]}$$
(2)

If the length and width of the channels is large compared with the borehole diameter, the flow-wetted surface may then be determined only as a function of the distance H, $a_R = 4/H$. Otherwise, L and W would be determined. W is not known unless independent observations have been made, e.g. in drifts and tunnels. The specific flow-wetted surface is not very sensitive to W and L (Gylling et al. (1997a)). Therefore, it may be obtained by interpretations of hydraulic packer tests.

4 Determination of the flow wetted surface. Numerical experiments

As discussed previously, a very important parameter for transport calculations is the flow-wetted surface. This is determined, as a first approximation, from the number of conductive fractures intersected by a borehole drilled in the site. However, the only information we may obtain from borehole data is the number of intervals (between packers) in which exist conductive fractures. For large fracture frequencies and large packer distances the probability that several conductive fractures are found in the same packer interval is high. The flow wetted surface calculated under these conditions may thus be strongly underestimated.

Borehole measurements are expensive, especially when a short packer distance is used. For this reason the number of boreholes drilled in the site would be small. In order to address these topics numerical experiments were performed. Hydraulic measurements in eight boreholes in Äspö, carried out with packer distances of 3 m, have been used as an experimental reference. Table 4-1 shows the number of intervals with conductive fractures for these boreholes. Two cut off are used for the hydraulic conductivity, $1.0 \cdot 10^{-12}$ and $1.0 \cdot 10^{-11}$ m/s. From these data, the mean hydraulic conductivity and the standard deviation of the hydraulic conductivity distribution were determined. Variograms were also made for each of the boreholes, a small or no correlation was found.

Borehole	Total number of packer intervals	Intervals with K>1.0 10 ⁻¹²	Intervals with $K>1.0\cdot10^{-11}$
KLX-01	198	198 (0.33)	194 (0.33)
KAS-02	235	233 (0.33)	199 (0.28)
KAS-03	151	151 (0.33)	149 (0.33)
KAS-04	109	109 (0.33)	107 (0.33)
KAS-05	129	129 (0.33)	105 (0.27)
KAS-06	163	163 (0.33)	157 (0.32)
KAS-07	164	164 (0.33)	161 (0.33)
KAS-08	159	158 (0.33)	119 (0.25)

Table 4-1Experimental borehole data in Äspö site. Numbers of intervals with
hydraulic conductivity larger than a given cut-off. The resulting
fracture frequency is found in parentheses.

	frequencies i	n the rock				
				Packer	Distance	
Fract./m.	m./fract.	2 m	3 m	5 m	10 m	30 m
0.1	10.0	11.0	11.5	12.8	16.0	31.4
0.2	5.0	6.1	6.6	7,9	11.6	30.2
0.3	3.3	4.4	5.1	6.5	10.5	30.1
0.5	2.0	3.2	3.9	5.5	10.1	30.1
1.0	1.0	2.3	3.2	5.0	10.0	30.1
2.0	0.5	2.0	3.0	5.0	10.0	30.1

Table 4-2Average distance between fractures obtained from hydraulic
measurements with different packer distances for different fracture
frequencies in the rock.

In the numerical experiments, a site with fractures randomly distributed in the rock is considered. The simulations are based on the assumption that a team drills a number of boreholes in the field. The total length of these boreholes is, for example, 4000 m. Once that the boreholes are drilled, hydraulic measurements are performed using different packer distances. From these "experimental" data the number of intervals with a hydraulic conductivity larger than the given cut-off is determined. In order to obtain reliable results, the experiment could be repeated a large number of times. The results (average values) are shown in Table 4-2. The spreading of the results between different "teams" was very small. If the distance drilled in the rock is reduced to 1000 m, the spreading of the results is somewhat larger (10-20 %).

The results in Table 4-2 are plotted in Figure 4-1. The ratio between the real H and the calculated H is plotted as a function of the ratio between the calculated H and the packer distance. H is the distance between fractures intersecting the borehole. The ordinate may be considered as a correction factor. From the hydraulic tests, the packer distance and the number of intervals with conductive fractures are known. From Figure 4-1, the correction factor may be determined.. The real value for H is then obtained by multiplying the calculated value of H by the correction factor.

From the figure, it may be observed that if the value obtained for H is much larger than the value of the packer distance, the correction factor is close to one and very stable. Small changes with variations in the ratio H/Packer distance. This may mean a very short packer distance and an expensive borehole. On the other hand, if the value obtained for H is close to the packer distance, the correction factor is close to zero. The corrected value for H will be affected by a very large uncertainty. For practical situations, values in the middle of the curve could be adequate, with no large uncertainty and not being too expensive.



Figure 4-1 Ratio between the real H and the calculated H as a function of the ratio between the calculated H and the packer distance.

5 Application case

The Channel Network model has been used to predict tracer tests, carried out within a 30 m cube scale experiment, in the TRUE (Tracer Retention Understanding Experiments) project. The TRUE project comprises of a series of flow and transport experiments performed at different scales. Simulations of the tracer experiments with sorbing solutes (STT1a) are shown below. True experiments were performed at the Swedish Äspö HRL at a depth of about 400 m (Winberg et al., (1996)).

5.1 Modelling of the TRUE experiment

The first stage of the TRUE project involved interference tests, dilution tests, flow loggings, pressure build-up tests and preliminary tracer tests. After this, several tracer tests with non-sorbing solutes were carried out in Feature A. Radially converging flow geometry and dipole flow were used in these tracer tests.



Figure 5-1 Feature A, the boreholes, the tunnel, and the niche. Behind Feature A some of the Feature B planes may be seen. For visualisation purposes the fractures are limited in extension. The boreholes KXTT1, KXTT2, KXTT3, KXTT4 and KA3005A are called T1, T2, T3, T4 and K5, respectively.

The code CHAN3D, based in the Channel Network model, was used in the modelling of the TRUE experiments. The results from previous tracer experiments with non-sorbing tracers were used to calibrate the transport model. In the flow model, the tunnel with the niche, all the boreholes, the Feature A and the Feature B planes were included. The conductances of the channels that connect the rock with the tunnel and the niche were reduced to simulate a skin effect. The size of the modelled rock volume was 30 x 30 x 40 meters in the direction longitudinal to the tunnel, the horizontal direction and the vertical direction respectively. This geometry is shown in Figure 5-1.

5.2 Modelling of the tracer experiments with sorbing solute

Several tracers were injected in the borehole section KXTT4. The water extraction occurs in borehole section KXTT3 with a flow rate of 400 ml/min. The injected sorbing tracers were Na, Sr, Rb, Ca, Ba, and Cs in ionic form. In order to avoid very long breakthrough times tracers with weak sorption properties were chosen. Figure 5-2 shows the breakthrough curves for the conservative tracer uranin and the sorbing rubidium.

In general, the breakthrough times for the sorbing tracer was longer than the predicted value. This may be due to that the value for diffusion in the rock matrix and sorption properties were based upon granite samples from intact rock. In experiments carried out

for quite short times, the tracer only has contact with the matrix close to the fracture. The tracers may also interact with filling material in the fractures. Filling material and the rock matrix close to the fracture usually show larger values for sorption and diffusion (Tullborg (1997))



Figure 5-2 Cumulative mass arriving to the extraction section for one realisation.

6 Discussion and conclusions

The Channel Network model has been used to simulate the tracer tests in the TRUE project. In this paper the application of the model to tracer tests with sorbing tracer is shown.

Numerical experiments were performed in order to address the data gathering for determining the flow-wetted surface. The results shown that the distance used between the packers has a large impact on the determination of the flow wetted surface. Packer distances smaller than the expected distance between fractures intersecting the borehole yields a better estimate of the flow wetted surface. However, the borehole measurements are very expensive if a too small packer distance is used. On the other hand, if the packer distance is similar or larger that the distance with which the fractures intersect the borehole the value of the flow wetted surface is determined with a large uncertainty.

The ratio between the "real" distance and calculated distance with which fractures intersect the borehole has been plotted. This ratio could be used as a correction factor since the ratio between the calculated distance between fractures intersecting the borehole and the packer distance are known from borehole measurements.

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GEOMASS: GEOLOGICAL MODELLING ANALYSIS AND SIMULATION SOFTWARE FOR THE CHARACTERISATION OF FRACTURED HARD ROCK ENVIRONMENTS

M. J. White¹, J. P. Humm¹, N. Todaka², S. Takeuchi² and K. Oyamada³

1. QuantiSci Ltd, 47 Burton Street, Melton Mowbray, Leicestershire, UK

2. PNC Corporation, Tono Geosciences Centre, Gifu-Prefecture, Japan.

3. JGC Corporation, Yokohama, Japan.

ABSTRACT

This paper presents the development and functionality of a suite of applications which are being developed to support the geological investigations in the Tono URL. GEOMASS will include 3D geological modelling, 3D fluid flow and solute transport and 3D visualisation capabilities.

The 3D geological modelling in GEOMASS will be undertaken using a commercially available 3D geological modelling system, EarthVision. EarthVision provides 3D mapping, interpolation, analysis and well planning software. It is being used in the GEOMASS system to provide the geological framework (structure of the tectonic faults and stratigraphic and lithological contacts) to the 3D flow code. It is also being used to gather the geological data into a standard format for use throughout the investigation programme.

The 3D flow solver to be used in GEOMASS is called Frac-Affinity. Frac-Affinity models the 3D geometry of the flow system as a hybrid medium, in which the rock contains both permeable, intact rock and fractures. Frac-Affinity also performs interpolation of heterogeneous rock mass property data using a fractal based approach and the generation of stochastic fracture networks. The code solves for transient flow over a user defined sub-region of the geological framework supplied by EarthVision.

The results from Frac-Affinity are passed back to EarthVision so that the flow simulation can be visualised alongside the geological structure. This workflow allows rapid assessment of the role of geological features in controlling flow. This paper will present the concepts and approach of GEOMASS and illustrate the practical application of GEOMASS using data from Tono.

1 Introduction

One of the principle mechanisms for the transport of radionuclides from a repository to the surface is the movement of groundwater. Understanding groundwater flow through the sub-surface geological environment is thus a key requirement of site characterisation activities. Developing this understanding requires characterisation of the geological structure and setting; and the acquisition and modelling of hydrogeological information. However, these aspects of site characterisation are commonly treated separately during site investigations and a need to make site characterisation data more accessible for modellers has recently been recognised by Geier (1997).

In hard fractured rocks the principal groundwater pathway for the migration of radionuclides are the fractures within the rocks. This has led to the development of a dual approach to modelling groundwater flow in which the regional flow is calculated using porous medium approaches and local flow is modelled by fracture network modelling techniques (e.g. Nirex, 1997). Both the integration of these approaches and the conceptual approaches used in the modelling have well-known shortcomings. Firstly, in a pure porous medium approach there are difficulties in representing the fast flow channels or preferential pathways due to fractures and faults. Secondly, pure fracture network models fail to account for any flow in permeable parts of the intact rock in which the fractures are located, which means that the simulated flow is critically dependent on the connectivity of the fracture network.

In order to overcome both the problems of the lack of integration of geological and hydrogeological investigations and the limitations of standard porous medium or fracture network modelling a new software system, GEOMASS (GEOlogical Modelling, Analysis and Simulation Software), has been developed for application at the Tono research centre in Japan. This paper describes the GEOMASS system and presents results from testing of the code.

2 Overview of the GEOMASS System

The workflow for the GEOMASS system is illustrated in Figure 2-1. The system provides software solutions for three aspects of the characterisation of hard fractured rocks. Firstly, the EarthVision geological modelling system provides the capability to construct 3D geological models and provides a suitable environment for the organisation of geological data into a standard format for interpretation, visualisation and analysis. Secondly, fluid flow is simulated using Frac-Affinity. Frac-Affinity is a code which allows the user to simulate three-dimensional flow in a heterogeneous, fractured rock.

The main new feature in Frac-Affinity is that it adopts a "hybrid medium" approach to the representation of fractured rock, which includes both permeable, intact rock and fractures. Thirdly, visualisation of the output from Frac-Affinity against the geological models is provided by EarthVision visualisation routines.

2.1 Geological Modelling using EarthVision

Geological modelling systems are families of software programmes which allow the construction of integrated 3D models of site investigation data, including subsurface geology, surface geography and engineering features. These systems concentrate on the development of static models which aim to produce a descriptive representation of the surface and subsurface and thereby provide the user with the ability to increase his understanding of the area of interest and to predict away from data locations.

3D geological models are commonly built by combining a structural framework with information on rock and fluid properties (e.g. porosity, hydraulic conductivity, fluid density or hydrochemistry) which have been interpolated away from data locations. The structural framework consists of 2D surfaces which represent stratigraphic boundaries or discontinuities (e.g. faults, fractures and dykes). In EarthVision, 2D surfaces are represented by a regular xy grid in which the elevation z is defined as a variable at each xy point. Property interpolation in EarthVision is undertaken onto a 3D array of points in which the 3D array is treated in a manner analogous to a 2D grid.

In order to test the integration of the GEOMASS system 3D geological models were constructed of the Tono area at a number of scales. These included a regional model encapsulating the drainage divide which is 12.21 x 11.23 km (Figure 2-2) and a local model centred around the area of site characterisation data which is 4.725 x 2.45 km (see Figure 2-7). The Tono area is underlain by a large Cretaceous granite pluton (the Toki Granite, Figure 2-2). Overlaying the unconformity surface at the top of the granite are a series of Miocene basins which host uranium mineralisation. The Mizunami Basin (see Figure 2-7) is the site for the Tono URL. This basin is offset by a reverse fault named the Tsukiyoshi Fault (see Figure 2-7).

The first step in the construction of the geological models was to organise the geological data into a standard format for integration and modelling of surfaces. A series of protocols and working practices were designed in order that the model construction process could be fully traceable and that subjective decisions could be recorded within the database. These protocols were based around three principles. Firstly, all data was collected into a sub-directory of the database to record the data in the form it was collected. Secondly, file naming protocols were adopted which allowed any user of the

system to identify a file easily. Thirdly, description logs were added to the file headers to describe the generation and use of each file within the database.

The geological models were then constructed by generating grids for each surface represented in the geological model, defining the topological relationships between the grids (by constructing a file called a *sequence file*) and then using the programs within EarthVision to integrate the grids and build a visualisation file. The geometry of the grids for each surface were controlled by the input data. Where the input data were sparse extra data were interpolated or shape transfer procedures were used to guide the gridding process. The sequence file used to define the geological models is a critical part of the GEOMASS workflow, in that it controls the construction of the geological models and the construction of the flow simulation grid.

2.2 Flow Simulation using Frac-Affinity

The basic idea behind the hybrid medium approach is represent a volume of fractured rock as two main components: "discrete features" and "intact rock" (Figure 2-3). Discrete features are objects such as faults or fractures that introduce linear/surface variations in the properties of the rock. A distinction is made between "deterministic discrete feature" which are relatively large scale features whose geometry might be determined accurately by a regional geological investigation, and "stochastic discrete features" which are the smaller scale fractures about which partial information may be interpreted from core logging or mapping (Figure 2-4). The intact rock is the remaining rock which is either completely intact or only contains "micro-fractures".

An additional feature of the hybrid medium approach is that it incorporates spatial variability in the properties of the intact rock and discrete features, both as a result of stratigraphy and more local heterogeneity. The stratigraphy is accounted for by using the output from the geological modelling as the framework in which rock properties are distributed. The local heterogeneity is simulated using geostatistical and fractal methods to generate interpretations of borehole data.

Properties of the intact rock are most naturally thought of as being associated with a volume (a "cell"). The approach adopted in Frac-Affinity is therefore to populate the cells in a grid with flow properties (conductivity, porosity and specific storage coefficient) which may be different in different stratigraphic zones. The rock properties may be uniform or spatially variable in different stratigraphic zones and may also be conditioned on borehole data.

Properties of the discrete features are more naturally associated with channels inside the features. The approach adopted in Frac-Affinity is therefore to generate a network of flow channels. In the large-scale deterministic features this is undertaken indirectly, by first gridding the feature's surfaces, and then identifying the equivalent network. In the stochastic features, the flow pathways network is identified directly.

Initially, the intact rock, deterministic discrete features and stochastic discrete features are handled separately. They must however be "merged" to form a hybrid medium. The approach adopted in Frac-Affinity is to convert the intact rock grid to an equivalent flow network, so that the representations of the three components of the hybrid medium are comparable. The three networks can then be joined, although particular care must be taken in handling the connectivity within and between the three networks, since the connectivity of pathways plays a key role in flow. A visualisation of a full hybrid medium network is illustrated in Figure 2-5.

Frac-Affinity is accessed using the Frac-Affinity Interface in either input or output mode (Figure 2-1). Both the input and output modes of Frac-Affinity are controlled by command-line prompts. The input mode of the Frac-Affinity Interface is used to define the geological structure and hydrogeological properties, and the boundary conditions and flow solver controls used in the simulation.

Frac-Affinity has been designed for application during the characterisation and operation of the proposed Tono URL. Therefore, the flow solver has the necessary conditions to simulate this scenario. These include time dependency, in terms of time dependent boundary conditions and hydrogeological parameters, and internal boundary conditions to simulate shafts and galleries.

2.3 Analysis and Visualisation of Flow Simulation Results

The output from Frac-Affinity is controlled by the Frac-Affinity Interface in output mode. The main outputs available from Frac-Affinity are; the intact rock and discrete feature properties; the head field across the model; monitor points, lines or planes at which the head values are output; flux planes; and pathlines. All of these outputs are output in a format suitable for importing either to a standard spreadsheet package or for visualisation and analysis in EarthVision. Two examples of the visualisation of Frac-Affinity calculation results are illustrated in Figures 2-6 and 2-7.

Figure 2-6 illustrates the calculation of the head field for the Regional Model. In this simplified example the boundary conditions were set to topographic, the east and west

boundaries were defined as no-flux planes and the hydrogeological parameters were set to uniform (the hydraulic conductivity being an order of magnitude higher in the sedimentary cover than the granitre basement). Figure 2-6 illustrates the effect of thickening of the sedimentary basins towards the centre of the model has on the head field.

Figure 2-7 illustrates the interpolation of heterogeneous rock mass properties on the Tsukiyoshi Fault in the Local Geological Model. In this instance the Tsukiyoshi Fault was modelled as a deterministic discrete feature. It can be seen from Figure 2-7 that the Tsukiyoshi Fault has been defined with boundaries inside the model region and this provides no difficulty within GEOMASS. Also visualised alongside the geological structure in Figure 2-7 is a schematic representation of a pathline. This pathline represents the tracking of a particle through the flow simulation with a data point output from the simulation each time the particle moves from one network node to another.

3 Discussion

The GEOMASS system provides a number of advantages over traditional approaches to the characterisation of hard fractured rocks for radioactive waste disposal. One of the most significant advantages of the GEOMASS system is the integration between the geological and hydrogeological interpretations of the site. The transfer of the geological framework model to the fluid flow network has been automated. Therefore, this process does not require the simplification of the geological framework (which can introduce artefacts into the simulation grid) and can be achieved within hours.

The rapid transfer of 3D geological interpretations for flow simulation allows the influence of the geological interpretation on the result of the flow calculation to be more readily assessed. This provides the ability for a number of different conceptual models of the geological and hydrogeological data to be investigated and the impact of geological uncertainty on the flow solution to be investigated.

The geological models provide significant added value to site characterisation. Firstly, they can be used as quantitative representations of the understanding of the site presenting the latest interpretation of all of the site features (3D geological framework; interpolations of rock mass (hydraulic conductivity, porosity etc.) and fluid (salinity distribution) properties; locations and trajectories of boreholes; borehole testing intervals etc.). These standard representations can be used as a basis for the analysis of a number of different aspects of the site. For instance, a consistent interpretation of the

geological structure can be used for 2D and 3D hydrogeological simulation if they are both derived from the same geological model. Secondly, the 3D geological models can be used to plan further investigations at the site (e.g. the drilling of boreholes based on an integration of the results of hydrogeological simulation with an interpretation of the 3D geological structure) and these further investigations can be predicted in advance.

The implementation of a hybrid model for hydrogeological simulation is also an important development within the GEOMASS system. This is a more realistic representation of the geological structure through which flow occurs and allows the calculation of porous and fracture flow mechanisms simultaneously. Therefore, the rock mass and fracture flow properties will control the flow solution not the connectivity of the fracture network. In addition, the development of Frac-Affinity overcomes the necessity of using a porous medium model for regional calculations and a fracture network model for investigations at the local scale. This has significant advantages in the development of integrated site characterisation studies.

It is intended that the GEOMASS system will be used throughout the investigations associated with the Tono URL. These include regional investigations into the geological environment; the construction of the shaft, including modelling, simulation and prediction prior to the shaft excavation; and the operation of the URL itself.

4 Conclusions

A 3D geological modelling, flow simulation and results visualisation system called GEOMASS has been developed to support the geological investigations at the Tono URL. The system allows integration of geological interpretation and fluid flow simulation. A new concept in fluid flow simulation, a hybrid medium representation which integrates intact rock and discrete features has been implemented in the 3D flow simulator Frac-Affinity. The GEOMASS system is available for the evaluation of the regional setting, excavation and operation of the Tono URL.

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Figure 2-2 Visualisation of the geological model of the Tono Region area. The model area is 12.21 x 11.23 km and it contains four stratigraphic units and four faults.



Figure 2-5 Visualisation of the network nodes for a small number of nodes in the Local Model. The red nodes indicate stochastic discrete features, yellow nodes a deterministic discrete feature and the purple and blue nodes the intact rock.



Figure 2.6 Visualisation of the calculation of the head field. In this steady state model uniform hydrogeological parameters have been assigned to the stratigraphic units. The boundary conditions are topographic head, with no flux boundaries to the east and west.



Figure 2.7 Visualisation of the Local Model (with simplified stratigraphy), with heterogeneous properties mapped on Tsukiyoshi Fault and a schematic representation of the visualisation of pathlines alongside the geological structure.

SELF-CONSISTENCY OF A HETEROGENEOUS CONTINUUM POROUS MEDIUM REPRESENTATION OF A FRACTURED MEDIUM

A R Hoch, C P Jackson, S Todman AEA Technology, Harwell, Oxon, UK

Abstract

For many of the rocks that are, or have been, under investigation as potential host rocks for a radioactive waste repository, groundwater flow is considered to take place predominantly through discontinuities such as fractures. Although models of networks of discrete features (DFN models) would be the most realistic models for such rocks, calculations on large length scales would not be computationally practicable. A possible approach would be to use heterogeneous continuum porous-medium (CPM) models in which each block has an effective permeability appropriate to represent the network of features within the block. In order to build confidence in this approach, it is necessary to demonstrate that the approach is self-consistent, in the sense that if the effective permeability on a large length scale is derived using the CPM model, the result is close to the value derived directly from the underlying network model. It is also desirable to demonstrate self-consistency for the use of stochastic heterogeneous CPM models that are built as follows. The correlation structure of the effective permeability on the scale of the blocks is inferred by analysis of the effective permeabilities obtained from the underlying DFN model. Then realizations of the effective permeability within the domain of interest are generated on the basis of the correlation structure, rather than being obtained directly from the underlying DFN model.

A study of self-consistency is presented for two very different underlying DFN models: one based on the properties of the Borrowdale Volcanic Group at Sellafield, and one based on the properties of the granite at Äspö in Sweden. It is shown that, in both cases, the use of heterogeneous CPM models based directly on the DFN model is selfconsistent, provided that care is taken in the evaluation of the effective permeability for the DFN models. It is also shown that the use of stochastic heterogeneous CPM models based on the correlation structure of the effective permeability is self consistent, provided that the distributions of the effective permeability and the spatial correlation of the effective permeability are approximated well.

1 Introduction

In many countries, the currently preferred option for disposal of radioactive waste is burial in a deep underground repository. At many of the sites that are, or have been, under investigation as possible locations for a repository, groundwater flow in the potential repository host rock is considered to be predominantly through discontinuities or fractures. For example, in the UK, the site that, until recently, had been under investigation by Nirex was at Sellafield, West Cumbria. The proposed host rock for a repository at Sellafield was the Borrowdale Volcanic Group (BVG), and an extensive programme of site characterisation focusing on the BVG has been carried out there (Chaplow, 1993). In Sweden, the proposed host rock for a deep underground repository would be granite. Experimental studies of groundwater flow in granite have been carried out at the Stripa Mine (Olsson et al., 1994) and at the Swedish underground research laboratory at Äspö (SKB, 1996). Investigations of groundwater flow in granites have also been carried out in the Swiss waste disposal programme (Thury et al., 1994). In BVG and granites, groundwater flow is considered to be predominantly through discrete discontinuities.

Models of groundwater flow through networks of discrete features (DFN models) would therefore be the most realistic and detailed models for groundwater flow in such rocks. However, in almost all cases, calculations on a regional scale using DFN models with every fracture represented would not be computationally practicable. The alternative to the use of DFN models is to use continuum porous medium models (CPM models), although recognising that the underlying model is one of groundwater flow through discrete features. Regional-scale calculations for CPM models are computationally practicable (see e.g., Nirex, 1997) for suitable choices of the size of the finite elements, or finite-difference grid-blocks, in the numerical model.

It is considered by many that the most appropriate CPM models to represent an underlying DFN model would be heterogeneous models, in which each finite element, or finite-difference grid-block, in a numerical calculation has an effective permeability appropriate to represent the network of features carrying flow within it. The correlation structure of the heterogeneous permeability field would then be implied by the underlying network. Such heterogeneous models would better represent the uncertainty about the hydrogeological behaviour of the system than homogeneous models.

A priori, this approach is reasonable. However, it is desirable to build confidence in the approach. In particular, it needs to be demonstrated that the approach is self-consistent, in the sense that, if the effective permeability on a much larger length scale than the elements in the heterogeneous model is derived using that model, then the result is close to the value derived directly from the underlying network model on the same length scale.

Self-consistency has been addressed by La Pointe et al. (1995) in a study based on the properties of Swedish granite at Äspö. This study apparently found that the proposed approach was not self-consistent. However, as recognised by La Pointe et al., there

were some deficiencies in their study. In particular, for the blocks in the heterogeneous CPM model, only the components of the effective permeability tensor parallel to the coordinate axes were considered. This leads to a very poor representation of blocks in which the main flow path entering the block leaves by an adjacent face rather than the opposite face. The effective permeability assigned to such blocks may be essentially zero, even though the flow paths through the block may contribute significantly to the overall flow through the network.

In this paper, the results of a study of self-consistency are presented for two underlying DFN models:

- the 'connected' model for the BVG that was used in the Nirex 97 assessment of the performance of a repository at Sellafield (Nirex, 1997);
- a model for the granite at Äspö based on that used by La Pointe et al. (1995). (It was not practicable to use exactly the same model, because in particular, LaPointe et al. calibrated their model against data that were not readily available for this study. However, the differences are not considered to be significant.)

These models were used as the basis for the study because the rocks in question are among the best characterised low permeability rocks in the world, and in view of the earlier study by La Pointe et al., there was particular interest in using the model for the granite at Äspö. The two models are quite different. In particular, on the length scales considered in the two cases, the model for the granite at Äspö is not as well-connected as the model for the BVG.

2 Analyses

The analyses of self-consistency carried out for each model had two main stages. In the first stage:

- a realization of the DFN model was generated in a suitably large domain;
- the effective permeability of the domain was calculated using NAPSAC (Hartley et al., 1996a);
- the domain was divided into many subdomains, and the effective permeability calculated for each subdomain from the relevant part of the DFN model in the large domain;
- a CPM model was set up in which each subdomain had the effective permeability determined from the corresponding subdomain in the DFN model, and the finite-element groundwater flow and transport program NAMMU (Hartley et al., 1996b) was used to calculate the effective permeability of the large domain;
- the effective permeability of the domain determined in this way was compared with that obtained directly from the DFN model in order to see if the proposed approach is self-consistent for this model;
- self-consistency on intermediate length scales was addressed in a similar way.

This first stage addressed the self-consistency of using a heterogeneous CPM model in which the effective permeabilities of the subdomains are obtained from the corresponding subdomains of a DFN model for the domain of interest.

However, in general it would not be practicable to generate realizations of the DFN model for all the corresponding rock in a regional model. One might therefore try to develop a stochastic heterogeneous CPM model in which realizations of the model were generated on the basis of the correlation structure for the effective permeability on the scale of the blocks in the CPM model, rather than being obtained directly from the corresponding subdomains in a DFN model covering the whole domain of interest. The correlation structure would be inferred by analysis of the effective permeabilities calculated for subdomains of a DFN model for a suitably large domain. Again, it would be desirable to demonstrate that the approach is self-consistent. A second stage of analysis was undertaken to examine this issue.

In this stage:

- the correlation structure of the effective permeabilities for the subdomains considered in the first stage of analysis was estimated;
- realizations of the heterogeneous CPM model for the large domain were generated directly on the basis of this correlation structure;
- the effective permeabilities of the large domain were calculated for each realization;
- the distribution of the effective permeabilities of the large domain was compared with the distribution of effective permeabilities obtained directly from realizations of the DFN model in order to examine the self-consistency of the approach.

3 Calculation of effective permeabilities

The approach adopted for the calculation of the effective permeability of a block within a DFN model was as follows. A 'guard zone' of a suitable size was chosen around the block. For several different directions, the residual pressure (effectively the head) corresponding to a uniform gradient in each direction was specified on the outer boundary of the guard zone. Then the residual pressure and the groundwater flows in the conducting features in the domain within this boundary were computed. The total flow through each face of the block of interest was calculated. The effective permeability tensor was determined as the anisotropic permeability tensor that gave the best overall fit to the flows for the different gradient directions.

This approach has several benefits. A full permeability tensor is calculated, not just the diagonal components. This helps to ensure that a non-zero effective permeability is obtained in the case in which the fractures only connect one face of the block to an adjacent face, rather than the opposite face. If only the diagonal components of the permeability tensor were calculated from the flow from one face of the block to the opposite face (as in the study of La Pointe et al.) then the effective permeability determined for such blocks would be zero, even though in the context of the overall DFN there could be significant flow though the block in question.

Secondly, the use of the guard zone helps to prevent the effective permeability for a block being biased by highly transmissive features that are not connected beyond the block, or are only connected to features with low transmissivity. If a guard zone were not used, then the effect of a highly transmissive feature connecting one face of the block of interest to an adjacent face would be as follows. Because of the imposed

residual pressure gradient, there would be a significant head difference across the feature, which would lead to significant flows and hence to a relatively high effective permeability for the block. However, in the context of the overall network, the head difference across the feature would be low (because of its high transmissivity) and the flow through the feature would be low. The approach adopted helps to ensure that (for a sensible choice of the size of the 'guard zone') the network in the block in question is behaving as it does in the environment of the overall network, which is considered to be very important.

4 Analysis for the BVG

4.1 First stage

By numerical experimentation, it was found that a suitable thickness for the guard zones for the DFN models of the BVG was 100 m. The study of self consistency for the model of the BVG was carried out for a block with side 800 m, which was subdivided regularly into subdomains with side 400 m, 200 m and 100 m. The effective permeabilities of a block with side 800 m were calculated for ten realizations of the DFN model. It was found that there was very little variation between the results for the different realizations. Results for one realization are given in Table 4.1. Thus, a block with side 800 m is, for practical purposes, a Representative Elementary Volume (REV) for this model, although not necessarily for the BVG at Sellafield.

The effective permeabilities for a block with side 800 m were also calculated using a heterogeneous CPM model in which each 100 m block had the effective permeability determined from the corresponding subdomain of the DFN model. The results are given in Table 4.1. There is good agreement, demonstrating self consistency. Similar studies were undertaken for blocks of side 400 m and 200 m subdivided into subdomains with side 100 m. Good agreement was found between the effective permeabilities calculated from the heterogeneous CPM models and the corresponding DFN models (see Figure 4.1). This demonstrates self-consistency on intermediate length scales.

4.2 Second stage

The correlation structure of the effective permeabilities of blocks with side 100 m obtained from the DFN model was analysed. The analysis was complicated. The permeability tensor for a subdomain has effectively six components, which are correlated, because they are derived from the same fractures. There are spatial correlations between the components for one subdomain and those for nearby subdomains, because the subdomains may have common fractures. Also, one would like to work in terms of the logarithm of the permeability, because permeabilities are often taken to have log-normal distributions. However, the off-diagonal components may be negative, so that the logarithm cannot be calculated.

The following approach was found to give a reasonable description of the correlation structure. The logarithms, P_1 , P_2 , P_3 of the principal components and three Euler angles α , β , γ defining the directions of the principal axes were calculated. Variables

 $D_2=P_1\mathchar`-P_2$, $D_3=P_2\mathchar`-P_3$

were introduced. Then transforms, P_1^* , D_2^* , D_3^* , α^* , β^* , γ^* , of the variables were defined such that the distributions of the transformed variables would be close to normal. It was found to be necessary to introduce the transformed variables, because the untransformed variables had very long tails on the side of low permeability values. Figure 4.2 illustrates the correlation structure of the transformed variables. It was found that

- P₁* could be approximated by a Gaussian spatial process with an isotropic exponential covariance with a length scale parameter of about 69m, corresponding to a range of about 200m;
- D₂* and D₃* could be approximated as linear combinations of P₁* and pure nugget processes;
- α^* , β^* and γ^* could be approximated as pure nugget processes.

Realizations of the permeabilities were generated by generating realizations of P_1^* (using TBCODE (Morris, 1998)) and realizations of five independent pure nugget spatial processes. Realizations of P_1^* , D_2^* , D_3^* , α^* , β^* , γ^* were obtained by taking appropriate linear combinations of the generated processes. Then the mappings leading to P_1^* , D_2^* , D_3^* , α^* , β^* , γ^* were inverted.

It was found that the effective permeabilities obtained from stochastic heterogeneous CPM models were in good agreement with those obtained from the DFN model, which demonstrates self-consistency for the use of stochastic heterogeneous CPM models.

5 Analysis for the granite at Äspö

5.1 First stage

A similar analysis to that for the BVG was carried out for the granite at Äspö. Because of the different length scales for the model of the granite at Äspö, domains an order of magnitude smaller were used in this case. It was found that there was considerably more variability between the effective permeabilities of the large blocks (with side 80 m) in this case, that is an 80 m block is not an REV (for the model used).

In Figures 5.1, effective permeabilities calculated from the heterogeneous CPM model and the underlying DFN model are compared for blocks of different sizes. It can be seen that there is generally good agreement, except for a small number of realizations for the smaller blocks, in which the DFN model had zero effective permeability. (For the purposes of plotting, the effective permeability of the DFN model was set to 10^{-20} m² in these cases.) This demonstrates self-consistency over the range of length scales considered.

In Figure 5.1, the results of LaPointe et al. (1995) are also plotted. It can be seen that the results of LaPointe et al. apparently suggest that the approach of using heterogeneous CPM models to represent a DFN model is not self-consistent. This is a very different conclusion to that reached in this study. It is considered that the
difference is due to the different approach adopted by LaPointe et al. to the calculation of effective permeabilities.

5.2 Second stage

The second stage of the analysis for the granite at Äspö was even more complicated than that for the BVG, for two reasons. First, the effective permeability of about half of the subdomains was zero. Second, there was significant variability between the different realizations of the DFN model. In order to address the first issue, an indicator approach was used to characterise the subdomains with zero effective permeability. In order to address the second issue, the correlation structure for each of ten realizations of the DFN model was analysed separately. It was found that a reasonable approximation to the correlation structure could be obtained by expressing the transformed variables as linear combinations of two Gaussian spatial processes with isotropic exponential covariances and pure nugget spatial processes, although there was an indication of anisotropic structure in some realizations. Each realization of the permeability was generated in a similar manner to that used for the BVG, and then a realization of the indicator variable was generated and the permeability was set to zero for the subdomains specified by this.

It was found that the distribution of the effective permeabilities obtained from the stochastic heterogeneous CPM models was in good agreement with that obtained directly from the underlying DFN model (see Figure 5.2), which demonstrates self-consistency.

6 Conclusion

This study has shown that the use of heterogeneous CPM models to represent a DFN model is self-consistent for two very different DFN models, one based on the BVG at Sellafield, and one based on the granite at Äspö. This has been shown both for heterogeneous CPM models in which the effective permeabilities of subdomains are obtained directly from the underlying DFN model and stochastic heterogeneous CPM models based on the correlation structure of the effective permeability. This builds considerable confidence in the use of heterogeneous CPM models to represent DFN models.

It was necessary to adopt a suitable approach for calculating the effective permeabilities of DFN models. It is considered that the approach described here of using a guard zone and calculating all the components of the effective permeability tensor is a good pragmatic approach. The use of guard zones means that, as far as possible the DFN model in a subdomain is behaving in the same way as the corresponding network in the overall model, and helps to avoid the results being biased by highly transmissive features that would not carry much flow in the larger network. Taking all the components into account means that a non-zero effective permeability is obtained for blocks in which fractures only connect adjacent faces. It is considered that the apparent finding of LaPointe et al. that the use of heterogeneous CPM models is not selfconsistent for the granite at Äspö is due to the different approach they adopted to the calculation of effective permeabilities. This is likely to lead to both under- and overestimates of the effective permeability. Indeed, they note that the use only of diagonal components may have had a significant effect on the results.

In the case in which stochastic heterogeneous CPM models based on the correlation structure of the effective permeabilities are used, it is very important to have a good approximation to the correlation structure. It is particularly important to develop a good approximation to the distributions of the components of the permeability tensor. It is not adequate simply to develop approximations that match the mean and variance.

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Table 4.1 Comparison of the effective permeability tensors (only upper half shown
for clarity) calculated for the first realization for the CPM model and
the DFN model of the block of BVG with 800m sides.

Effective permeability (m ²) for the DFN model			Effective permeability (m ²) for the CPM model		
1.24 10-16	-1.23 10 ⁻¹⁷ 1.88 10 ⁻¹⁶	-5.14 10 ⁻¹⁸ -7.33 10 ⁻¹⁷	1.36 10-16	-1.52 10-17 2.04 10-16	-8.03 10 ⁻¹⁸ -8.40 10 ⁻¹⁷
		1.97 10-16			2.09 10-16



Figure 4.1 Comparison of the k_{11} component of the effective permeability tensors obtained from the CPM model for blocks of BVG with those obtained directly from the underlying DFN model.



Figure 4.2 Some of the covariances of the transformed variables P_1^* , D_2^* , D_3^* , α^* , β^* , γ^* for the first realization of the model of the BVG.



Figure 5.1 Comparison of the k_{11} component of the effective permeability tensor obtained from the heterogeneous CPM model of blocks of granite at Aspö with that obtained directly from the DFN model. The results from this study are shown by solid circles. For comparison, the results obtained by La Pointe et al. (1995) are shown by open circles on the plot for the 80m block. (For a few realizations of the smaller blocks, the effective permeability of the DFN model was zero. For the purposes of plotting, the effective permeability of the DFN model was set to 10^{-20} m² in these cases.)



Figure 5.2 Comparison of the distributions of the k_{11} component of the effective permeability obtained directly from the DFN model for the granite at Äspö with the distribution obtained from the heterogeneous CPM model based directly on the underlying DFN model and the distribution obtained from the stochastic heterogeneous CPM model based on the correlation structure of the effective permeabilities of the subdomains. The mean and estimated 95% confidence interval of the values plotted are also shown.

EFFECTS OF ICE MELTING AND REDOX FRONT MIGRATION IN LOW PERMEABILITY MEDIA

Jordi Guimerà, Lara Duro, Salvador Jordana and Jordi Bruno QuantiSci S.L. PTV 08290-Cerdanyola (Barcelona, Spain) jguimera@quantisci.es

Abstract

Migration of oxidising groundwater could adversely affect the ability of deep repository systems to limit radioelements releases to acceptable levels. Glaciation-deglaciation periods enhance the presence of deep oxidising water, thus jeopardising stable chemical conditions of the repository over a long period. We assess in a quantitative basis the possibility of such oxidising front to happen, by using limited regional groundwater flow schemes with heterogeneous models. We consider that the consumption of oxidants under the soil cover will be governed by the reactions between groundwater and redox buffering minerals. The ability of the media to buffer an oxidant intrusion will be dominated by the presence of iron(II) bearing minerals such as chlorite, biotite and pyrite. The ability of clays containing Fe(II) to act as oxidant sinks has been pointed out by several authors. Our study approaches the problem under two perspectives: equilibrium approach, where groundwater reaches equilibrium with minerals able to release Fe(II), and kinetic approach, where the interaction between oxidants and the minerals is not instantaneous, but governed by kinetic rate laws. Results show that, while the equilibrium approach is applicable whenever groundwater residence times are sufficiently long, kinetically controlled reactive transport gives more accurate results, provided that characteristic reaction times are longer than groundwater residence time. Multicomponent reactive transport results show that despite the glacial origin, groundwater remains anoxic after periods of thousands of years and the redox state is governed by the presence of iron in the system. We have performed a sensitivity analysis of the effects of varying the groundwater flow velocity, the available reactive surface and the presence of minerals. The majority of the simulations indicate that the resulting geochemical composition of the system would not jeopardise the stability of the spent fuel, at repository depths. Consequently, the intrusion of melting ice water does not pose any threat to the chemical stability of the repository system at the depths considered in the SKB concept.

1 Introduction

The Swedish concept of deep geological disposal of nuclear spent fuel is based on geologic environments under reducing conditions. The inflow of oxidising groundwa-

ters to critical depths could adversely affect the ability of engineered and natural barriers to limit radioelement releases from the disposal system to acceptable levels. A safety assessment exercise (SKI SITE 94) considers that a sequence of glaciation-de-glaciation periods could induce the presence of deep oxidising water, thus jeopardising the chemical stability of the repository. In this context, studies performed in the Fennoscandian shield indicate the presence of isotopically light water, of glacial origin, within major fracture zones at depths down to 400 m (Outokumpu case, Blomqvist et al., 1992; Glynn et al., 1997).

This work assesses quantitatively the consequences of the penetration of an oxidising front due to the infiltration of de-glaciation water. We will proceed with a number of assumptions and simplifications, due to the complexity of the problem and the uncertainties associated to some critical parameters and conditions.

Water infiltration due to de-glaciation will last for approximately 5000 years (Björck and Svensson, 1992). The next major glaciation is expected to occur in about 60000 to 75000 years. The melting rate can be extrapolated from present measurements that indicate some 50 mm/year (Boulton et al., 1995 in Svensson, 1996), however, it is not clear how long it will last and which are the expected fluctuations of such a rate.

The data concerning oxygen content in ice sheets and in ice melting water has been taken from research projects in polar areas -Antarctica and Greenland- and other glacial areas. Most of the data from polar programmes concerns the stable isotopic composition of ice, information on oxygen and major components contents in melt water is less abundant.

The reductive capacity of the system (RDC) will be mainly given by minerals which alteration will release reductants such as Fe(II). Pyrite, biotite and chlorite are reasonable candidates. Their thermodynamic evolution in contact with groundwater is rather well established. However, the knowledge about their kinetic alteration is far more limited and some assumptions have to be taken in order to perform the reactive transport calculations.

The problem is approached by two different methods. First, whenever the residence time of groundwater lasts longer than the characteristic reaction time (groundwater velocity, v <3 m/y) water-rock interactions are assumed to be governed by thermodynamic controls. In this case, the geochemical evolution of the system is assessed by using the PHREEQC code (Parkust, 1995) with the associated databases. Also, the stationary-state approach (Lichtner, 1988) is attempted.

For faster groundwater velocities (v>3 m/y), as equilibrium cannot be assumed for the main water-rock interactions, we have performed reactive transport simulations to couple groundwater flow and the kinetically controlled geochemical system. The reactions are assessed by means of the ARASE code (Grindrod et al., 1994).

2 Conceptual model

The geology of the target area consists of fractured rocks of low permeability in top of which, advance and retrieval of ice sheets takes place. The depth of the repository is estimated to be 500 m below surface. The host rock is divided into two regions which are geochemically different: an upper one, where redox conditions are likely to be oxidising, extending down to 100 m below surface, and a lower one of 400 m thick which reaches the repository top. Groundwater redox conditions are reducing in this latter zone, in accordance with the data from the Äspö site and other site characterisation programmes. The system considers hydraulic steady state during a period of some 1000 years (Svensson, 1996).with a infiltration rate around 50 mm/year. The oxygen content in ice is estimated to be 1.4 mM (about 45 mg/l, pe = 11 to 13, Ahonen and Vieno, 1994).

We start by defining the system as 1D. The system is viewed as a column of two different materials: an upper part of oxidising conditions and a lower one which is reducing. The reducing capacity of the top soil due to the presence of organic matter and microbial activity is not taken into account, although some studies showed that it is not negligible in this context (Banwart et al., 1995). The infiltrating water is considered to be in redox equilibrium with the oxidising bedrock; consequently, reactive transport simulations are carried out in the reducing zone, where the evolution of the redox front is presumed to display more variability.

The problem has also been approached in 2D. For that, the flow field has been varied to reproduce the most likely real flow conditions. In spite of the limitations of the multicomponent reactive transport codes, different material zones simulating fractures, host rock and reducing and oxidising conditions have been included.

The redox state in granitic groundwaters is governed by electron transfer between Fe(II) and Fe(III) aqueous and mineral species. Therefore, the largest reductive capacity of such systems will be given by the iron(II) content. The occurrence of iron(II) in nature is dominated by minerals such as Fe(II) sulphides, carbonates (siderite) and clay minerals. White and Yee, (1985) propose an structural oxidation of Fe(II) in which Fe(II) is oxidised without being released to the aqueous phase. Also homogeneous Fe(II) oxidation has been reported, in which Fe(II) is released in the form of Fe²⁺ from the clay and it is subsequently oxidised to Fe(III) in solution (Malmström et al., 1995).

A potential repository will be located in a reducing zone in which mineralogy changes according to the water flowing fractures and the host-rock. Chlorite represents a 35% of the fracture coating in the fracture fillings of Äspö, with an average content of 20% wt. in FeO (Banwart et al., 1995). Chlorite can be regarded as a solid solution whose endmembers are Daphnite ($Fe_5Al_2Si_3O_{10}(OH)_8$) the ferrous end-member, and Clinochlore, the magnesian end-member. We have assumed that it behaves ideally and, according to the calculated stoichiometry, the following solubility constant has been used:

Chlorite14A (Fe_{1.5}Mg_{3.5}Al₂Si₃O₁₀(OH)₈) + $16H^+ = 1.5Fe^{+2} + 3.5Mg^{+2} + 2Al^{+3} + 3H_4SiO_4 + 6H_2O$ (1) with logKso = 59.9

Pyrite and biotite are the most abundant iron (II) rich minerals in the host rock. Biotite can be regarded as a solid solution whose end members are Annite (ferrous, KFe₃AlSi₃O₁₀(OH)₂) and Phlogopite (magnesian). We have considered an ideal solid solution of these two end members to generate the biotite phase:

Biotite $(KMg_2AlFeSi_3O_{10}(OH)_2) + 10H^+ = K^+ + 2Mg^{+2} + Al^{+3} + Fe^{+2} + 3H_4SiO_4$ (2) with logKso = 35.88.

3 Preliminary calculations

The equilibrium approach considers that the extent of oxygen consumption is limited by the equilibrium state. For that, the PHREEQC code (Parkhust, 1995) has been used and the system is envisaged as two compartments: oxidised and reduced zone. The oxidised zone considers as initial groundwater the shallow groundwater reported by Banwart et al. (1995) equilibrated with calcite and $Fe(OH)_3(s)$. The reduced zone considers native Äspö groundwater as initial groundwater.

Fractured media simulations assume that chlorite oxidises and it produces $Fe(OH)_3(am)$. In order to keep controlled the chemistry of the system, the precipitation of clinochlore has been allowed. Thus, the system behaves as if the structural iron of chlorite is being released to the system and equilibrated with $Fe(OH)_3(am)$. For host rock calculations equilibrium with pyrite and biotite was assumed. In this case, both minerals are able to accept oxidants and to precipitate in the form of $Fe(OH)_3(am)$.

The oxic intrusion is buffered by the dissolution of chlorite in the fractured medium. The pH evolves from 7.7 to 8.3 and the initial pe (-2) slightly increases due to the equilibration of the system with chlorite (final pe = -1.07). The dissolution of chlorite gives rise to a precipitation of Fe(OH)₃(am). In the host rock simulations the oxic intrusion is buffered by biotite and pyrite and the chemistry of the system is very efficiently buffered to a pH of 8.27 and a pe of -4.37. The redox effect exerted by biotite is negligible if pyrite is present in the system.

Although the equilibrium approach is efficient at understanding the system, it presents severe limitations since it assumes that the water replacement is complete. Therefore, the validity of the approach largely depends on the number of cells considered. Another limitation is that water is assumed to equilibrate with the minerals present in the system which is valid only when the characteristic times of reaction are lower than the residence times of groundwater. Therefore, it can lead to important misinterpretations when considering dissolution of aluminosilicates (such as chlorite and biotite) or sulphides (e.g. pyrite) due to their slow kinetics of dissolution under most natural groundwater conditions.

4 Multicomponent reactive transport model

An advantage of the use of multicomponent reactive codes is that both hydrodynamics and geochemistry are lumped together, so as enabling to envisage a problem under a more reliable approach. The counterpart is that the numerical problem solves thousands of equations at every time step. As a result, the CPU times may become impractical. Therefore, it is advisable to reduce the number of variables which are not dominating the geochemical system and to use domains as simple as possible to optimise the performance of the problem. In order to do so, preliminary calculations are an efficient way to constrain the model. Thus, the weathering equations of the minerals participating in the RDC of the system (chlorite, biotite and pyrite) have been reduced to a function of Fe(II) release which is dependent on pH in the case of the silicates and on the oxygen content in the case of pyrite. Also, the number of thermodynamic equations has been reduced to less than 20.

Measured groundwater compositions in the Äspö site and in Antarctic research programmes were used as initial and chemical boundary conditions respectively. As regards to parameters and water composition, the first have been kept as close as possible to realistic values either by using field measurements (Rhén et al., 1997) or expected values during glaciation periods (Boulton and de Marsily, 1997).

Some 30 cases were analysed in 1D by combining hydrodynamic parameters (basically, groundwater velocity), type of mineral and its reactive surface. Figure 1 summarises the most relevant results. At first glance, we observe that the arrival time depends on the groundwater velocity and that the magnitude of the redox front -that is, the final pe value- depends on the surface area of the mineral considered. Despite the relevance of the first arrival time of the redox front, we observe that the effect of groundwater velocity on the final pe value is important when the mineral is assumed to dissolve independently on the state of saturation of the system. In this case, differences of one unit pe are obtained. On the other hand, when the kinetic rate law depends on the saturation index, i.e., when the rate of dissolution decreases as the system approaches equilibrium, then the final pe values are exactly the same.

In all the calculations the dissolved oxygen concentration obtained is lower than 10^{-30} mol/l at relatively early times. This has two main implications: First, that the oxidants of the system will not be those entering within the melting water, but the ones resulting from the subsequent water rock-interaction processes. Second, that at this low oxygen contents pyrite does not contribute to the reductive capacity of the system, because its kinetics of oxidation is directly proportional to the oxygen content. Therefore, the effects of the advance of the oxidant front have to be analysed in terms of the evolution of the reductive capacity (RDC) of the system. Differences in dissolved Fe⁺², which is the dominant aqueous contributor to the RDC, are usually small, - 6.75×10^{-5} mol/l -. The dissolution of chlorite becomes null far from the oxidant boundary. Moreover, after 100 years the system reaches saturation and a slight precipitation occurs (few milimoles).

Six cases were analysed in 2D according to different flow field configurations. Main differences relied on the groundwater residence times down to depths of the repository, since a considerable part of water flows through the top oxidising zone in some of the cases, without affecting the repository depth. In terms of the consequences for the performance of the repository, the most conservative simulations showed variations of the RDC comparable to those produced in 1D (see Figure 2).



Figure 1. Comparison of the evolution of pe at repository depth for different cases. Different minerals and reactive surface areas are compared across the graphs.

The resulting pe either hardly displays any variation or it attains values up to 4-5. Consequently, the RDC of the system at certain locations barely changes or decreases down to 4 orders of magnitude. This latter would be the case where downward flow is considered along a highly transmissive fracture (Figure 3, groundwater velocity around 10^{-5} m/s, which by no means reflects "low permeability").

5 Implications for safety assessment

The arrival of oxidising fronts within a glaciation time span is feasible. An oxidant mass balance is indicative of the real threat of the geochemical conditions for the repository. For this purpose, we use the fracture distribution measured at Stripa (Abelin et al., 1991) and we attribute a certain oxidant mass flow to the various fracture types. Thus, $Fe(OH)_3(aq)$ is the relevant oxidant in solution and its cumulative mass flow reaches values up to 10^{-8} mol/m² after 1000 years. Only very fast flowing fractures - groundwater velocities on the order of 10^{-5} m/s - produce a dramatic change in the redox state of the interface geosphere-near field. We should not expect to place the repository under such a fracture and consequently the chances for this negative case can be dismissed by proper site characterisation.

6 Conclusions

A quantitative analysis of redox front advance in a granitic environment due to melting of ice during deglaciation periods has been done. To evaluate the consequences we have used the following three approaches: the stationary state, the system is in equilibrium with redox buffering minerals and the dissolution (weathering) of such minerals happening at a slower rate than groundwater flow. The hydrogeochemical systems considered have been: preferential flow through fractures, where the redox system isdominated by the presence of chlorite and flow through the host rock, where the dominant reducing minerals are biotite and pyrite.

The equilibrium approach is fairly optimistic since pressumes that the whole mineral content is available for groundwater interaction, and reacts until equilibrium is reached. Accordingly, the redox front progresses slowly and oxidising conditions do not reach the repository depth in a million years period. The equilibrium calculations showed the differences exerted by the minerals considered on the migration velocity of the redox front. For instance, in the host rock environment, pyrite becomes determinant while the effects of biotite are less important.

The multicomponent reactive transport approach showed the relevance of two items: the reactive surface area (S_A) and the velocity of groundwater. S_A determines the pe value at which steady state is reached and the velocity controls the time at which certain steady state is reached (it may well be that such state is not reached). Dispersion became relevant in terms of first arrival times but it was not crucial in terms of final values of the redox state. Hydrodynamic conditions are conservative given that, in general terms, most of the cases assume relatively fast groundwater velocities. On the contrary, the geochemical perspective is slightly optimistic: we consider that all the mineral content is available to reaction, that reactive surface area does not vary with time neither with the extent of dissolution, and the formation of a protective coating formation is not taken into account.



Figure 2. Evolution of the Fe(II) species in a 2D model at repository depth when about half of the melt water flows by the top zone and half down to repository depths with considerable flow along and across a fracture zone. Note that Fe⁺² is the main species contributing to the RDC of the system. Below: Point 3 pertains to a fast flowing fracture, while the rest are located within the host rock



Figure 3. pe profiles at different simulation times for host rock and fracture respectively. Note that the top 100 m (from 500 to 400m) are the oxidising zone and the repository altitude is 0.

The effects of the oxidising front migration has been analysed in terms of variation of the reduction capacity (RDC) of the system given that minerals dissolution is negligible in most of the cases. Thus, Fe^{+2} is the main contributor to the RDC. The cases analysed show that RDC in the host rock barely changes due to that oxidant mass flow is small too. On the contrary, changes up to four orders of magnitude are found in fractures. Such difference between host rock and fractures has been corroborated by means of oxidant mass balance as well. This is important since if a decrease of the release of reductants - in terms of coating phenomena or reactive surface area diminishing - were accounted for, redox conditions at the repository level could be more oxidising.

In terms of safety assessment analysis neither of the cases considered could seriously jeopardise the geochemical conditions of the repository system, in spite of the fast velocity or the relatively small reactive surface area adopted for some of the runs.

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Session 3

Integrated characterization of potential repository sites and URLs – application in performance assessment and siting

EXPERIENCE GAINED FROM THE SITE CHARACTERISATION STRATEGY USED AT THE ÄSPÖ HARD ROCK LABORATORY

Göran Bäckblorn

Swedish Nuclear Fuel & Waste Management Co, Sweden (Presently at Power Reactor and Nuclear Fuel Development Co, Japan) e-mail: gb@tono.pnc.go.jp, skbgb@skb.se, Fax: +81-572-55-0180

Abstract

The Äspö Hard Rock Laboratory is a "dress-rehearsal" facility to test, develop and demonstrate technology and models prior to applications at the actual deep repository site in Sweden. Site characterisation methodology has for more than a decade been a main issue at the Äspö Hard Rock Laboratory (HRL).

At the start of site investigations in 1987 the following strategy was adopted:

- Comprehensive surface and surface-based investigations
- Multi-disciplinary data collection in batches
- Staged integrated evaluations on selected key issues closely tied to existing knowledge of the geology of the site
- Iterative modelling on several geometrical scales based on existing (scarce) data
- "Predictive approach" to model updating

During the Construction Phase of the Äspö HRL (1990 - 1995), a multitude of data was collected to test and to increase the details of the models made prior to construction.

Several things have been learned regarding the appropriateness of the adopted approach to site characterisation. These findings concern e.g. data collection methods from surface and underground, construction/test-integration, choice of useful and feasible model concepts, data flow and document management.

The acquired understanding, knowledge, skill and know-how are very valuable for planning useful and feasible site characterisation for the deep repository in Sweden.

1 Introduction

Site data for a deep geological repository are essential to develop the scientific understanding of the site, to engineer the repository, to assess the environmental impact and the long-term post-closure safety. The approach used at Äspö to test the reliability of the site characterisation methodology was to iterate the data-model-prediction-outcome-evaluation chain through a multi-disciplinary approach. The models were structured to different key issues and geometrical scales to allow for co-ordination and integration of data collection, modelling and evaluation.

Site characterisation for the underground research laboratory began in late 1986. Four years 1986-1990 were devoted to investigations from ground surface and from boreholes. Models of rock conditions at depth were developed and further detailed during the following five years (1990 - 1995) when the laboratory was constructed. Data collected in the 3.6 km long tunnel down to a depth of 450 m, in surrounding boreholes and in boreholes drilled from the tunnel were evaluated and compared with predictions based on the pre-construction models. The paper Bäckblom et al,(1997a) provides an overview of the work conducted. The summary report Rhén et al,(1997), Chapter 8 and Bäckblom et al,(1997b) are the documentation of some general experiences gained from the site characterisation. This paper discusses some of the experiences gained focussing on the general approach for the site characterisation.

2 Site characterisation for the Äspö HRL and for a repository. Similarities and differences

The approach used at Äspö and at a future repository site will not be identical. Some similarities and differences are discussed.

2.1 The general context

Site characterisation is a technical issue, but will have to adapt to the social and political environment as well. The friendly social environment at Äspö has not put any constraints on the scientific-technical programme, what activities to conduct or where to locate boreholes. To mitigate the environmental impact, the local politicians favoured a design change of the facility having consequences for the site characterisation. Influence from the social and political environment on site characterisation is foreseen for the repository case as well.

The system optimisation process - site properties-engineering-scenario evaluation is a more complex undertaking for the repository case than for the previous scope of works at Äspö. In the case of a repository, site characterisation is a part of the work to evaluate the technical suitability of the site. Such a site provides a good potential

• for the engineered barrier system to completely contain the waste for a very long time. The most important requirement is the general long-term favourable and stable geological environment,

- to construct, operate and seal the repository accordingly to set specification, to conduct site investigations to obtain understanding of the site and its interaction with the engineered barriers, to analyse the safety of the system and compliance with regulations,
- to retard and dilute any nuclides at the time the containment function of the engineered barrier system is not available.

The work at Äspö 1986- 1995 has been focussed. One important aspect of the studies was to test the ability to obtain a thorough understanding of rock conditions based on surface-based site investigations.

2.2 Scientific understanding

The objective to gain a scientific understanding of the geological environment of the site is an important overall ambition for the work at the Äspö HRL and it will also be important for site characterisation at the repository site. The stage goal set to *demonstrate that investigations at the ground surface and in boreholes provide sufficient data on essential safety-related properties of the rock at repository level* however led to a somewhat narrowed scope. It was thought to be necessary to use a "predictive approach" to the model updating. The predictive approach has many distinct advantages, but also drawbacks, c.f. Section 4.2. One important narrowing of scope was that predictions were basically made only for such issues that were possible to update during the construction phase. This focus implicitly led to data collection close to the tunnel and data collection for subjects where the data during construction phase will provide additional information. Scope of works not addressed explicitly is e.g. consequences of future glaciation, regional groundwater flow and evolution of the site with time, thermo-mechanical issues etc. The work conducted at Äspö does however provide a good basis for the ongoing extended studies during the Operation Phase.

2.3 Engineering

The Engineer shall design an Underground Research Laboratory and a repository facility so that it is safe and environmental during construction, operation and that post-closure safety is assured for the case of the repository. In the case of repository engineering it is foreseen that several, now lacking design requirements will need to be developed. Site properties of importance for emplacement of canister, buffer, backfill and plugs should be established. The work initiated at Äspö to study the effect of heterogeneity on selection of e.g. suitable canister positions, Rosén, Gustafson, (1995) is a step in the right direction. In hindsight, additional work could have been done earlier to set up explicit models coupling site data with engineering consequences for e.g. grouting, reinforcement. Several exciting theoretical and practical developments were now carried through during the construction phase. Can we be trusted making long-term predictions of the system if we make poor descriptions of the engineering issues that could lead to unexpected engineering challenges during repository implementation?

2.4 Performance Assessment, Safety Analysis

During implementation of the repository it is likely that the successive detailed design decisions will be supported by Performance/Safety Assessment (PA, SA). Current PA, SA is biased to post-closure assessment of a repository without design flaws for the time period after

re-saturation. Requirements on occupational safety and the practicability of engineered barrier emplacement, may require rock support and/or sealing by grouting. The effects of such measures on post-closure performance are not explicitly evaluated in the PA, SA. It is logical to find a site that makes it possible to fulfil the assumptions in the PA, i.e. - no rock support/sealing in the near-field - should not PA treat such engineering measures. There are many system requirements to control. PA, SA is an incomplete feasibility control of all the system requirements, focussed on the important issue the long-term radiological safety.

It would have been beneficial for the work at Äspö HRL and for the work to develop practical PA if a hypothetical repository analysis had been carried out as a part of the Äspö works. One of the aims should be to develop PA to an efficient tool to support the detailed engineering decisions. The Swedish authority SKI has recently published their Deep Repository Performance Assessment Project SITE-94, SKI, (1997). A hypothetical KBS-3 repository was placed at Äspö. The PA conducted was based on the pre-construction Äspö data. Such studies are highly important as input to further develop site characterisation methodology. One essential aspect is the transparency of data, analysis, models and evaluations. SKB and SKI have found areas where improvements in data management are useful for efficient evaluation of the future repository site.

2.5 Environmental Impact Assessment

A significant issue with respect to an URL and a repository is the assessment of environmental impact. The environmental impact is to an extent dependent on choice of engineering alternative. It is important to select the engineering to be reasonably robust also with respect to pre-closure environmental impact as well. The flexibility shown by SKB in the Äspö HRL siting stage when the environmental impact really was an issue is highly recommendable. The complete re-design of the entrance of the access tunnel from Äspö to the Simpevarp area was really necessary to reduce the environmental impact and to obtain necessary permits for construction. The basic understanding acquired by the comprehensive site characterisation was crucial to make a reliable environmental impact assessment. Can we be trusted making good long-term predictions of the system, if we make poor assessments of the environmental impact during construction and operation of the facility?

2.6 Conclusion

Site characterisation for the Äspö Hard Rock Laboratory and for the repository shows more similarities than differences. The differences noted so far are to a great extent due to the fact that the goals for the Äspö HRL and the repository site characterisation are not identical.

3 Integration of the multi-disciplinary site characterisation.

The establishment of an underground research laboratory and a geological repository is a complex undertaking. This includes, but is not limited to permits, site characterisation, integrating construction and research activities and carrying out complex high-quality research in underground conditions. Good integration of site characterisation is a part of the quality management. Integration necessitates participants willing to integrate and having efficient methods for data, analysis, modelling and evaluation at hand. The Webster Dictionary

definition of the concept integration are e.g. to form into a whole, to unite with something else, and to end the segregation of. Some planning considerations for the Pre-investigation Phase and the Construction Phase are highlighted: The goals of the work have gradually been refined. There was a strong commitment to find the most relevant objectives "What is the right thing to do?" There was a strong commitment to Project Management - keep Quality, Time and Cost. Specific tasks not executed within the set frames were used as indicators to identify areas for improvements. There was a strong commitment to Team Building with a few Scientific Principal Investigators with clear but broad responsibilities. The contractors chosen for the construction of the underground facility viewed the project as a research project with construction, not as a construction project with some research that was added.

Site characterisation generates a huge amount of data, models and reports. The reporting style chosen for the Äspö project is quite cumbersome, both to generate and later to digest for the readers. What has been a heavy responsibility burden for the Principal Investigators are the integrated evaluation reports. They take time to produce and it takes time to have them sufficiently mature. An alternative approach could be viable where shorter Technical Notes in a Work Breakdown Structure-fashion are favoured. These Technical Notes and other documentation should be transparently tied to a powerful and versatile database equipped with excellent visualisation capability. The documents should of course be available on cd-rom or formatted for Intranet/Internet.

Integration will never be complete, but "*I hear and I forget, I see and remember, I do and I learn*". The provisional checklist provided in Table 1 can be used to find out in areas for improved integration. The checklist is based on experience on matters that promotes and hampers integration of site characterisation.

4 Evaluation of the iterative approach

An iterative approach to data-models-prediction-outcome evaluation has been tested as a part of the Äspö site characterisation approach. This approach is in general advantageous and applicable for the repository site characterisation as well. The repetitive approach can be used to test that data are reproducible, that concepts still are valid after gaining further data and to optimise site characterisation, engineering and the performance assessment. It was a conscious choice at Äspö to make "models" as the basic product of the work. The overall idea is that the models should be useful and feasible for application in the real repository case.

4.1 What aspect of the model is tested?

The basic products from the Äspö site characterisation are "models". The models were made for lithology, geological structures, mechanical stability, groundwater flow and groundwater chemistry. Scoping calculations were made for models on transport of solutes. The models were made on different scales to account for different level of detailing etc. Constructive comments by the Äspö Scientific Advisory Committee led to development of a standardised format for describing the models, Olsson et al (1994).

The most important iteration -closely connected with the stage goal to verify preinvestigations - was considered to be comparison of models before and after construction of the laboratory using a predictive approach to modelling. During the site investigations - prior to construction -16 holes were cored and 20 percussion holes were drilled with a total length of 7,4 km and 2,4 km respectively. During the construction phase 60 cored holes and 404 percussion holes were added totalling 6,6 km and 8,6 km respectively. The data collected during the construction phase were mainly to check and detail the models set up prior to construction. In hindsight further work could have been done to explain how the results from the iterative site characterisation was to be applied in the model updating.

An overall important aspect is that iteration is used to build additional understanding and confidence in the underlying processes. An example is the redox conditions. The iterative site characterisation at Äspö HRL confirmed the reducing conditions in the bedrock, but identified a new process -microbiology - as a contributing factor.

According to the model definition, Olsson et al, (1994) a model consists of two parts, one part is the concept and the other part is the data. It should be clarified if the iteration is made to test the appropriateness of the concept, to test the ability to make reliable parameter estimation or if the intention is the combined test of the concept AND the ability to make reliable parameter estimation. Many models at Äspö intended to show that there existed a useful and feasible concept to describe a process and that appropriate parameter estimation was achievable in a realistic geological setting. For some models (e.g. draw-down of the groundwater table, inflow to shaft etc.) the outcome is however very dependent on the construction process. The outcome will change if the layout change, if grouting is done etc. It is thus not enough to make a model consisting of the concept and data, but ALSO to predict how the Engineer will decide the technical solution and the outcome of the technical work. The successive engineering of the facility to the local rock conditions will thus be in conflict with the predictive approach favouring no changes to facilitate evaluations of the predictions. The predictive approach helps to establish consistency and transparency but is not flexible. It is thus contra-productive to use a predictive approach during the construction phase.

In the iterative approach to model updating, it should be clarified whether iteration is made to update the output of the model, the boundary conditions, the spatial assignment of parameters, the material properties, the geometrical framework or to increase confidence in the past, current or future processes. Many aspects of the model can be updated without direct coupling to the construction schedule. A recommendation is to decide subject by subject how updating efficiently should be dealt with. The early choice of nomenclature and definitions in the project is quite important. The way this work is done is quite decisive for definition of model concept, that later will be updated and refined. Re-definition and re-classification at a later stage hampers transparency.

The differences between updating deterministic and stochastic models are appreciated. For the stochastic models it is important to decide whether the sampled distributions are representative of the site. For some subjects at Äspö, like primary rock stresses, the parameter range assigned was too narrow, which was found out when additional data were collected.

4.2 Site characterisation constraints

In spite of extensive data collection there will always be uncertainty connected with the interpretations based on the data. The decision of how much data should be collected (and associated uncertainty tolerated) can be based on different types of constraints. A simple

constraint can be: Spend the amount of X, accept the uncertainty and make the decision, or Spend Y years of investigation, accept the uncertainty you gain and make the decision. It is also possible to put a statistical constraint on data collection: Continue the investigations until the mean error of model M is less then ε or a subjective condition, that is: Collect data until you are confident that you understand the site. It should be kept in mind that it is often more difficult to show non- existence of processes and features, "to show how things cannot be" than "to show how things are".

The amount of surface-based investigations at Äspö was basically determined by a time constraint. It was thought that four years of investigations were reasonable to deal with the issues at hand. The time constraint on site characterisation during the Construction Phase was very much tied to the progress of the excavation.

The detailed site-specific strategy can only be devised after some site investigations at the site have been carried out.

4.3 Conclusions

The iterative approach to model testing is useful, but it should clearly be stated what aspect of the model that is tested in the iteration. For the case of a repository, where like at Äspö, design of the facility should adapt to a technical, social and political process more flexible ways for model updating should be searched for. The predictive approach selected to test the models offers advantages, like clear systematic to the work, to establish consistency and transparency. The main disadvantage is that the approach is not flexible and for many of the models the outcome is very dependent on the construction process.

The detailed site-specific strategy, including constraints can only be devised after some site investigations at the site have been carried out.

5 Evaluation of modelling on different geometrical scales

The general approach to the site investigations was to work from regional investigations and focus on progressively smaller scales. After regional investigations and initial surface-based investigations in the Simpevarp area, models were made on several geometrical scales.

The Äspö site characterisation and supplementary studies have been sufficient to develop good regional models of past and current processes, features. The models have not been so critical for selection of present boundary conditions at Äspö since they are to a great extent controlled by the construction impact. For the repository case the regional models are important to decide boundary conditions necessary to extrapolate the performance of the sealed repository into the future time.

The focus on the investigations at Äspö has been on the so-called site-scale models (100-1000m) that are very important for siting, engineering and performance assessment of the repository. The approach to site-scale models has been useful and feasible.

The block-scale models and the detailed-scale models are important for evaluation of the potential of the near-field to protect the engineered barriers, to engineer the repository and to

assess the barrier retention capability. The current licensing situation for a repository in Sweden calls for block-scale models based on surface-based investigations. The confidence in the block- and detailed-scale models will be easier to develop in a more homogeneous geological setting than at the Äspö site. "Full" models linking output and input were not made for the block-scale (50-10 m) and detailed-scale models (0-5m). These models were basically conceptual and relating to parameter estimation. The block-scale models were made for predetermined positions along the planned access ramp, but a more flexible, stochastic approach would have been more useful. The block-scale models have been quite difficult to realise, due to the high lithological heterogeneity. Based on the surface-based site data available it would have been possible to advance the models in block-scale further. The data acquired step-wise during the pre-investigations and the construction phase can now be used to re-assess what could have been achieved at what stage in the investigations. The capability of realistic modelling has also advanced tremendously over the last ten years. This development is both conceptual as well as with respect to development of computer hardware and software. The Äspö site is quite heterogeneous and offers many possibilities to test, develop and demonstrate what level of certainty is possible to achieve in the block- and detailed-scale models. Such models will encompass issues like lithology, structural geology, mechanical stability, groundwater flow and groundwater chemistry but not the least the barrier retention function of non-sorbing and sorbing species.

6 Evaluation of the issue resolution capability

The requirement set by SKB was to test the ability to obtain a thorough understanding of rock conditions based on investigations of the surface and investigations in and between boreholes. Based on this general requirement and on the requirement to design, construct and operate the facility with existing technology without major problems a set of key issues and key subjects were developed. The Äspö HRL summary report, Rhén et al, (1997), c.f. Table 8-1, discusses the subject resolution capability with respect to scientific understanding, site-specific knowledge that has been arrives at Äspö and also usefulness and feasibility of methods.

Site characterisation in conjunction with construction work at Äspö has basically confirmed the pre-construction models. However the models - as expected - have become more detailed after the construction period. The work at Äspö has shown that such pre-construction models can be obtained for the studied key issues through the application of "standard methodology of good quality" for measurements, data analyses, modelling and evaluation. Areas have been identified where further development of techniques and methods would be useful.

With respect to scientific understanding local variability of rock stress, rock burst, scale dependency of hydraulic conductivity, the detailed groundwater flux within small volumes of the rock and the excavation disturbed zone are areas for further studies. Site-specific knowledge was obtained for a range of subjects, but to a lesser extent where the scientific understanding is limited. Due to the heterogeneity it was not possible to describe the local variability of lithology nor the deterministic location, extent and properties of individual minor fracture zones. The spatial variability of parameters describing mechanical properties and rock stress were underestimated. Useful and feasible methods exist for a range of the subjects studied. Rock burst, local flow distribution and microbiology are examples of areas where improvements in methods are of interest.

7 Concluding remarks

The Äspö work has involved many researchers and experts offered an opportunity to test, develop and demonstrate understanding, knowledge, skill and know-how. Each of the participants has their own experience to share. The investment in intellectual capital at Äspö - both human and structural during the last ten years has provided valuable experience in most tasks required for characterisation of a repository site and the design and construction of repository facilities in crystalline rock. Site characterisation has been adequate and reliable for engineering purposes. For safety assessment purposes the site characterisation work at Äspö has provided comprehensive knowledge on geological, geohydrological and geochemical conditions in the rock mass. The work at Äspö has also included the development of a formal quality system for *in situ* measurements, interpretation and modelling.

Äspö is an established international centre for research and development in the field of deep geological disposal of nuclear waste. The international co-operation is stimulating and has promoted high quality and diversity in ideas and concepts. In addition, the results are made available to a larger international community, where they can be applied to different concepts for deep disposal of radioactive wastes. Some of the results at Äspö are site-specific, but quite a few of the results and experiences should be possible to generalise to the benefit for other waste management programmes.

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Table 1 Site Characterisation Integration Test Formula

ISSUE	Yes = O
GENERAL	110 - A
Team.cnuil?	
Team not too hig (Core group less than 10 persons)?	
Data-modelling-evaluation is iterative?	
All stens in the experiment are well-planned (including evaluation)?	
Results evaluated with respect to scientific understanding?	
Results evaluated with respect to application to repository engineering?	
Results evaluated with respect to application to performance assessment	
of a repository?	
Results evaluated with respect to application to site investigations for a	
repository?	
SCORE	
GOALS	
Product-oriented?	
Easy to measure when goals have been met?	
Detailed goals and stage goals in line with overall goals?	
Team members know the context for the work and	
the product oriented goals?	
SCORE	
DATA	
Units used consistent with the SI-system?	
Data are stored in a common x,y,z co-ordinate system?	
Objectives set for a multi-purpose drill hole?	
Priorities made for a multi-purpose drill hole?	
Measurement points located to cover the natural variability?	
Uncertainty in measurements recorded?	
SCORE	
ANALYSIS	
Nomenclature established for features etc.?	
Data stored in a versatile database?	
Data can be visualised in 3D?	
Schedules are set to allow for co-interpretation?	
Data from different disciplines are checked for consistency?	
Scale is taken into account?	
Conceptual uncertainties discussed?	
Uncertainty in analysis recorded?	
SCORE	

ISSUE	Yes = O No= X
MODELS	[
Concepts used are clearly stated?	
Assumptions made are clearly stated?	
Geometrical framework is clearly stated	
Input parameter data used clearly stated?	
Parametrization made transparent with respect to collected data?	
Algorithms for extrapolation/interpolation of data clearly stated?	
Boundary conditions clearly stated?	
Output of models clearly stated?	
Results consistent with expectations?	
Results consistent with other results from other disciplines?	
Software used is verified?	
Models stored in a versatile model database?	
Models can be visualised in 3D?	
SCORE	
CALIBRATION	
Location of monitoring points relevant?	
Measurement accuracy compatible to -or higher than needed-to measure the modelled anomalies?	
Procedures established for "good-enough"-fit?	
Data-flow streamlined so data formats are compatible?	
SCORE	
PREDICTIONS	
Is input (prediction) and output (outcome) defined?	
Will measurement methodology, instruments, evaluation procedures,	
scales etc. used to check predictions be the same as used to collect the	
data for the predictive models?	
Are methods established to compare prediction and outcome?	
SCORE	
EVALUATION OF MODELS/METHODS	
Are data checked for consistency and interrelation?	
Are "success criteria" established for evaluating deterministic/stochastic models?	
Are formats for documenting and sharing results established?	
SCORE	

USE OF SITE SPECIFIC DATA FROM ÄSPÖ - PRELIMINARY RESULTS FROM THE ON-GOING SAFETY ANALYSIS SR 97

Anders Ström SKB, Sweden

Jan-Olof Selroos SKB, Sweden

Johan Andersson Golder Associates, Sweden

Abstract

This paper discusses an on-going safety assessment study of the Swedish Nuclear Fuel and Waste Management Company (SKB) as well as the use of field data from Äspö for obtaining input parameters for flow and radionuclide transport modelling in the geosphere. In the on-going Safety Assessment study SR 97, three individual sites in Sweden are used for exemplifying site specific conditions on overall repository performance. Thus, models capable of reproducing site specific characteristics are utilised. This is primarily obtained by implementing the geologic structural models in suitable conceptual models for groundwater flow on both regional and local (site) scales. The models for flow incorporate observed and/or inferred water conducting features as well as other site-specific characteristics necessary for realistic descriptions of flow at the sites. The flow modelling thus aims at realism; the results obtained for present day conditions should not in any serious aspect conflict with observations (e.g., flow, pressure, mixing) at the site. Agreement between observed and modelled entities provides confidence in that a sound understanding of the site is obtained. Äspö is one of the three sites providing site-specific conditions in SR 97.

Transport is subsequently modelled using a streamtube approach where the "travel times", for nonsorbing species, and discharge locations of a set of one-dimensional streamtubes are obtained from particle tracking in the flow model. The resulting distribution of "travel times" in a single model realisation reflects the spatial variability and spatial extent of the repository, whereas the ensemble travel time distribution (over several realisations) for a given canister location reflects the uncertainty in travel time. The actual transport paths used in the transport modelling are thus dependent on site specific information such as e.g. existence of water conductive features. Other input parameters to the transport model are based on more generic and/or conservative arguments. However, the goal in a safety assessment context is to establish confidence in the modelling approach while showing compliance with regulatory standards rather than it is to convey perfect realism in every detail of all models used.

In general all data entered into the final assessment models have undergone several steps of modelling and interpretation. Hydraulic tests are interpreted by well test analysis. The information is analysed statistically, is upscaled and introduced into a stochastic continuum model. This latter modelling is used to derive migration paths and travel times. Variant cases may originate from ambiguities in data, but can only be formed by applying expert judgement. Also the matrix data is based on an expert selection where, as a minimum, the representativity of the data has been assessed. All final parameter selection also undergoes internal peer review. This implies that expert judgement is a necessary ingredient in parameter selection.

This paper is limited in the sense that SR 97 is an on-going safety analysis project. This means that integration, conclusions, feedback to site characterization and similar issues are still remaining. Thus, this paper will provide glimpses from the on-going project related to Äspö and the far field.

Introduction

At the present time SKB is involved in producing a new safety assessment study called SR 97 (Safety Report 97) for a deep repository for spent nuclear fuel. SR 97, which is part of a series of activities scrutinizing all pertinent aspects of deep-rock nuclear waste disposal, is primarily aimed at analyzing the long-term safety of a deep-rock repository in Sweden. New features of SR 97 as compared to previous analyses is that more emphasis is placed on the canister integrity and on systematic treatment of data uncertainties in radionuclide transport analyses. Furthermore, three separate locations in Sweden are analyzed in order to illustrate the site-specific conditions. The safety report, which is to be delivered early 1999, is a site-specific application of SR 95 /SKB, 1995/ which was a framework indicating how a complete safety assessment study should be performed.

Site specific conditions and model parameters related to the nearfield and engineered barriers are not specifically discussed.

Compilation of site specific information

The three hypothetical sites are named Aberg, Beberg and Ceberg, each of which is based on data from previous site characterisation studies conducted by SKB. These are:

- Aberg, which is based on the Äspö Hard Rock Laboratory in southern Sweden;
- Beberg, which is based on investigations at Finnsjön, in central Sweden; and
- Ceberg, which is based on investigations at Gideå, in northern Sweden.

Äspö is the most recently and thoroughly investigated site in the SKB program and is also the site of the intensive investigations associated with the Äspö Hard Rock Laboratory (HRL). Beberg is based on Finnsjön, perhaps the second-most thoroughly investigated site in the SKB program. Finnsjön was also the subject of SKB 91, a previous PA modelling study. The last site, Ceberg, is based on data taken from Gideå, one of the oldest SKB site characterisation studies. Although a great deal of data exists for Gideå, it is the least thoroughly investigated site of the three sites.

The actual flow and radionuclide modelling work for different scenarios in SR 97 is preceded by compilation of existing site specific data. For each discipline such as hydrogeology, hydrochemistry etc. a compilation is conducted of existing data and descriptions are made for each of three sites for use in modelling. Each compilation is intended to provide modelling teams with parameter values and uncertainties for inputs to numerical models on the regional and site scales. Specifically, for hydrogeology the compilation report /Walker, 1997/:

- reviews the investigations at the sites and existing reports,
- summarises the current knowledge of conditions and uncertainties regarding the hydrogeology of the sites,
- updates the data and analyses in order to correct known errors and inconsistencies, and
- provides estimates of the block-scale parameters for use in modelling of the sites at the regional and site scales.

Its primary objective is to provide consistent data sets so that the results of modelling will be as comparable as possible. One limitation of comparing modelling studies for alternative sites is that

the site characterisation studies and analyses of data are frequently conducted at different times for different goals. Although the bias and error of site investigations are never fully known, a consistent analysis of the data and presentation of conceptual models will at least help confine the differences to the sites themselves.

Geosphere modelling and parameters

SKB has traditionally in performance assessment studies used fairly sophisticated models for the description of spatial variability in primarily hydraulic properties. Stochastic continuum models on both regional and local scales have dominated in the performed safety assessment studies such as SKB 91 /SKB, 1992/. Discrete models have also been adopted, but mainly in more research oriented projects.

For SR 97, the flow modelling aims at realism; the results obtained for present day conditions should not in any serious aspect conflict with observations (e.g., flow, pressure, mixing) at the site. Agreement between observed and modelled entities provides confidence in that a sound understanding of the site is obtained. Transport is subsequently modelled using a streamtube approach where the "travel times", for non-sorbing species, and discharge locations of a set of onedimensional streamtubes are obtained from particle tracking in the flow model. The resulting distribution of "travel times" in a single model realisation reflects the spatial variability and spatial extent of the repository, whereas the ensemble travel time distribution (over several realisations) for a given canister location reflects the uncertainty in travel time. The actual transport paths used in the transport modelling are thus dependent on site specific information such as e.g. existence of water conductive features. Other input parameters to the transport model are based on more generic and/or conservative arguments. The specific one-dimensional transport code used, FARF31, incorporates advection and dispersion along the migration path, matrix diffusion combined with sorption and chain decay. The direct input parameters to FARF31 are the travel time tw, the flow wetted surface per volume of water aw, and the "Peclet-number" describing the relation between advective velocity times migration length and dispersivity as well as nuclide specific K_d-values and diffusivities of the rock matrix. In reality both the flow and the specific surface area vary along the migration path and it can be shown that proper equivalent parameters can only he obtained by integrating the quotient between the flow wetted surface per volume of rock and the Darcy velocity along the migration path. However, in SR 97 the approach is simplified by assuming flow wetted surface and porosity to be constant in space. Thereby, the groundwater flow input to migration modelling can be described in terms of the travel time distribution only.

The set of one-dimensional migration paths and travel times are obtained from three-dimensional flow modelling. The underlying conceptual model of the rock assumed is one of a rock domain described as a spatially varying stochastic continuum intersected by conductor domains (fracture zones), also modelled as porous media, but of hydraulic properties distinct from the rock domain. The approach further assumes a nested approach using a site scale model, with relatively much detail in conductive structures and adoption of a stochastic continuum model embedded in a regional scale model with less geometrical detail and with equivalent, i e non-stochastic, hydraulic parameters. The fractures zones are inferred from a geological structure model resulting from a joint interpretation of topography and surface and bore hole geophysical data. The majority of available information on the rock hydraulic conductivity is in the form of small scale (a few m), bore hole hydraulic tests. Data belonging to designated conductor domains are treated separately from data representing the rest of rock mass, thereby allowing for assignment of different hydraulic properties to these two classes. The data are treated as geostatistical samples and

resulting geostatistical properties are estimated and upscaled to the model discretization scale. There is no specific assessment of dispersion along migration paths; dispersivities are selected in a pragmatic way. The main dispersion in the system is handled by the difference between different migration paths.

Estimates of the flow wetted surface along migration paths is obtained by underestimating the conductive fracture frequency and noting that there is at least one conductive fracture in a flowing test section. This procedure is strictly valid only if the flow is evenly distributed between all paths, whereas in the general case it is necessary to integrate the flow width along the migration path. The approach is selected partially out of lack of more detailed information and partially due to limitations in present modelling tools. For the assessment this means that the potential errors need to be handled in the uncertainty evaluation.

A sub-project within SR 97 is the so called Alternative Modelling Project (AMP) aimed at quantifying conceptual model uncertainty. The specific objectives of AMP are thus to *illustrate rock barrier performance* using different conceptual models and to *assess model robustness* in terms of relevant far-field performance measures. Three different conceptual models of the spatially variable geosphere are used. These are a stochastic continuum model, a discrete fracture network model, and a channel network model. The different conceptualizations of the rock mass are illustrated in Figure 1. The stochastic continuum model used is HYDRASTAR; a code developed and extensively used within SKB /Walker et al, 1996/. HYDRASTAR is also used for the main modelling of SR 97 mentioned above.



Figure 1. Illustration of different conceptual models used for flow and transport modelling.

The choice of these three models in the AMP exercise is primarily based on the fact that all models have successfully been used in previous analysis of field-scale flow and transport experiments in Sweden. Thus, it is of interest to evaluate if models that all explain field data will result in significant differences when applied in PA applications.

In order to enable conditions which permit a quantitative comparison between the different conceptual models, it was early recognized that a clear project strategy and modelling specifications had to be defined. In the first phase of the project it was decided to emphasize on conceptual differences in flow related descriptions. It is believed that the analysis within AMP will be simplified by only comparing transport related parameters for use in FARF31 and COMP23 rather than comparing final results from individual transport codes. However, in future stages of AMP transport may be simulated directly by all three models.

It was also decided to use site-specific data from the Äspö Hard Rock Laboratory within AMP to the greatest possible extent. The site-specific data used pertains to discrete zones with known

transmissivity and conductivity statistics for the rock mass in between. Since parts of the geological data only is known in a statistical sense, multiple realizations of the spatially variable rock domain is to be employed. Furthermore, the boundary conditions used were obtained from a regional model for Äspö, and the canister locations coincide with parts of a hypothetical repository placed at Äspö within the SR 97 safety assessment study. A strong emphasis in AMP has been put on the definition of output entities to be calculated and subsequent performance measures for comparison of the output. A number of performance measures quantifying various aspects of the output have been formulated.

The evaluation of AMP is still on-going and no final results are available at the present moment. However, a few preliminary findings and conclusions may be reported. Our experience is that even though strict modelling specifications are defined, it is hard to safeguard that the different conceptual models actually address identically the same problem. This is primarily due to the fact that not every single aspect of the problem can be defined in the specifications, thus leaving room for individual judgment and decisions, which may be biased by the possibilities offered by the conceptual model utilized. Furthermore, the results obtained so far indicate that it may be hard to quantitatively compare e.g. absolute values of the travel times resulting from different models due to the different assumptions invoked. Rather, the span of travel times and corresponding uncertainties are more relevant for comparison.

Discussion and conclusions

This paper is limited in the sense that SR 97 is an on-going safety analysis project. This means that integration, conclusions, feedback to site characterization and similar issues are still remaining and so the paper cannot be very conclusive.

All data entered into the final assessment models have undergone several steps of modelling and interpretation. Furthermore, expert judgement is used in selecting structural models and variant cases for the flow modelling. Also the matrix data is based on expert selection; as a minimum the representativity of the data has been assessed.

The general approach to deal with parameters unlikely to be measurable is to try to simplify and apply conservative parameter values. The difficulty with the approach taken is that the conservatism can be criticised, but also that the resulting performance may be too pessimistic. The way to deal with this problem is on one hand to make sure that the parameter is not crucial to repository performance and on the other hand to search information indicating that indeed present parameter values are too extreme.

The results obtained in the alternative modelling project may have some consequences on SR 97 in general and on future safety assessments specifically. The main reason for applying different models is to address conceptual model uncertainty. A stronger confidence in the results is foreseen as a consequence of the use of multiple conceptualizations. It is emphasized that in the future, spatial variability in other than hydraulic parameters (e.g., parameters affecting radionuclide retention) may also be incorporated in PA analyses. Both theoretical model development and experimental work (at the Äspö Hard Rock Laboratory) are presently being performed in order to address such issues.

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THE USE OF SITE CHARACTERIZATION DATA IN THE NIREX 97 PERFORMANCE ASSESSMENT

C P Jackson and S P Watson AEA Technology, Harwell, Oxon, UK

Abstract

Over a number of years, Nirex examined the possibility of a deep radioactive waste repository at Sellafield. Extensive site investigations were carried out, using both surface geophysics and a number of deep boreholes. Hydrogeological measurements were carried out over a wide range of length scales. The work culminated in the Nirex 97 performance assessment.

The use of the site characterization data in Nirex 97 is described. The hydrogeological data can be divided into two main categories: direct measurements of the hydrogeological properties of the rocks on various length scales, and measurements of 'derived' properties such as groundwater head, salinity and temperature. The former data were used to derive initial values of the effective hydrogeological parameters for use in groundwater flow and transport models on various length scales. In order to do this, it was necessary to relate the measurements to the underlying variability and then upscale from the underlying variability to the length scales of interest. The quantification of the uncertainties, relating these to the available data, formed a major part of the analysis.

The models were then calibrated using the second category of data. This led, using a Bayesian approach, to revised characterizations of the uncertainty, which were used in the calculations of repository performance.

An important feature of the analysis is the systematic treatment of the uncertainties and their relation to data. When allied to an ongoing evaluation of the suitability of a site for a repository, this enables the key uncertainties to be identified as a focus for future site characterisation work.

1 Introduction

United Kingdom Nirex Limited is responsible in the UK for disposal of intermediatelevel and certain low-level radioactive waste. Between mid-1991 and March 1997, the Nirex programme considered the potential suitability of a site at Sellafield, West Cumbria as a possible location for a deep repository. An extensive investigation of a region around the potential site has been carried out using surface geophysical techniques, a number of deep boreholes and laboratory studies. In particular, hydrogeological measurements have been carried out over a range of length scales, from laboratory tests on core samples with length scales of a few centimetres to large scale cross-hole tests. The work culminated in the Nirex 97 assessment (Nirex, 1997) of the performance of a potential repository at Sellafield.

In this paper, an overview is given of the use of the site characterisation data in Nirex 97. Much of Nirex 97 was devoted to the analysis of the groundwater pathway, which is the main pathway by which radionuclides from waste in the repository might return to the immediately accessible environment. Therefore, data relevant to hydrogeology played a major role in the assessment and are the main focus of the discussion here. The hydrogeological data can be divided into two categories:

- direct measurements on various length scales of the hydrogeological properties of the rocks;
- measurements of 'derived' quantities such as groundwater head, salinity or temperature.

The direct data were used to provide initial characterisations of the uncertainty in the hydrogeological parameters for groundwater flow and transport models on various length scales. The measurements of derived quantities were used to calibrate the models and refine the initial characterisation of the uncertainties.

The analysis and processing of the data for Nirex 97 was a major task, not least because of the detail of the conceptual model for groundwater flow at the site and the large amount of data available. New techniques were developed to undertake the work, and advances in understanding were made.

2 Use of direct data

The direct measurements of hydrogeological properties on various length scales were used to provide an initial characterization of the uncertainties in the effective hydrogeological parameters for groundwater flow and transport models on various length scales. In order to do this, the measurements were first related to the variability in the hydrogeological properties of the rocks on the smallest length scales. Where necessary, a process of downscaling was used. Then the properties were upscaled to the length scales of interest, principally the regional scale. For example, for the repository host rock, the Borrowdale Volcanic Group (BVG), the main source of information on the transmissivities of the Flowing Features (FFs) that carry groundwater flow was a suite of Environmental Pressure Measurements for borehole intervals of about 50m length. These gave effective hydraulic conductivities, which generally resulted from several FFs. It was necessary to infer the distribution of the transmissivity of FFs. The effective permeability of the BVG was then determined from models of networks of FFs and clusters of FFs (Nirex, 1997).

Simple analytical models, that is models in which the quantities of interest are approximated by simple analytical expressions in the underlying parameters of the models, were used for most of the upscaling calculations. In the most important cases, the simple analytical models were supported by numerical models.

A key part of the analysis was a systematic treatment of uncertainties. These arise from various sources such as:

- measurement error;
- variability;
- uncertainties about the conceptual model;
- approximations made in modelling.

Variability leads to uncertainty because it means that the detailed variation of the rock properties cannot be determined by practicable measurements. Statistical descriptions that characterise the variation to an accuracy that depends on the number of measurements, the variability and its correlation structure can be developed. In Nirex 97, variability was quantified on three broad ranges of length scale:

- centimetres to metres;
- metres to hundreds of metres;
- hundreds of metres to tens of kilometres.

The uncertainties in the underlying parameters of the models were recognised and quantified and then propagated through the analysis, leading to a quantification of the uncertainties in the effective parameters. In this context, the use of simple analytical models was a very powerful technique, which enabled the uncertainties in the effective parameters to be estimated in a practicable manner. This was done using the First-Order Second-Moment Method (see for example, Dettinger and Wilson, 1981). One of the benefits of this is that it enables the relative importance of the uncertainties in the underlying parameters to be assessed in a very straightforward manner.

The end-product of the analyses was the initial characterization of the uncertainties in the effective hydrogeological parameters for regional-scale models (see Figure 2.1).

3 Use of derived data

In addition to the direct data, measurements of derived data, such as groundwater head, salinity and temperature were available. These data were independent of the direct data, and were used to calibrate the groundwater flow models, that is to determine ranges of hydrogeological parameters that lead to an acceptable match between observations and the corresponding quantities calculated using the models. Taking the additional
information provided by calibration into account leads (see Figure 3.1) to a revised characterization of the uncertainties.

A two-stage approach to calibration was adopted. In the first stage, parameter space was systematically searched (see Figure 3.2) to find a reasonably good match to all observations simultaneously. The variant that gave the best match in this stage was taken as the reference model for the next stage of calibration.

In the second stage, parameter space in the vicinity of the reference model was systematically explored to try to estimate the region of parameter space in which there is an acceptable, if not necessarily good match to observations (see Figure 3.2). This was done by varying one parameter at a time to find the constraints on the parameter in question. It should be emphasised that an acceptable match to all the observations simultaneously was sought. The decisions as to what was acceptable were made in a fairly conservative way, that is substantial deviations from the observations were allowed.

In comparing the observations and the corresponding calculated quantities, it was necessary to take into account:

- uncertainties in the data;
- the fact that the small-scale heterogeneity of the system was not represented in the model;
- for the two-dimensional model, the fact that many of the boreholes were not on the line of the cross section of the model.

The process of calibration is illustrated in Figures 3.3 and 3.4. Figure 3.3 shows the match to the environmental head in one of the Nirex deep boreholes for the two-dimensional reference model of Nirex 97. The Figure shows:

- the observed environmental heads and the associated uncertainties;
- a guideline that shows the key features of the data that it was desired to reproduce;
- the calculated environmental head for the two-dimensional reference model at the best location corresponding to the borehole;
- the calculated environmental head at locations either side of the best location that might still correspond to the borehole.

Figure 3.4 illustrates the second stage of calibration. The Figure shows the match to the environmental head in one borehole for the reference model and for variants in which one of the parameters of the model was altered in steps of half an order of magnitude, values both higher and lower than those in the reference model being considered. From this comparison, it was considered that all of the variants in which the parameter was increased were acceptable, but of the variants in which the parameter was decreased, only the first was acceptable. This provided one of the constraints from calibration.

The information about the parameters obtained from calibration was combined with the 'prior' information obtained from upscaling using a Bayesian approach (see for example, Cox and Hinckley, 1974). Various technical complications needed to be addressed. In some cases, it was recognised that the match to the data would not be affected if all the hydrogeological parameters were scaled by the same amount. For example, the match to the head and salinity data for a steady-state model with boundary

conditions, as in Nirex 97, that are either prescribed head or no-flow is not significantly affected if all the effective permeabilities are scaled by the same amount. Another complication was that there were prior correlations between the uncertainties in various effective hydrogeological parameters. Such correlations arise because the parameters in question depend to some extent on the same data.

These complications were handled by approximating the constraints from calibration by normal distributions. These were then combined appropriately with the prior distributions that characterised the uncertainties, which were also approximated by normal distributions. This led to revised normal distributions that characterised the posterior uncertainties. The analysis involved straightforward, but lengthy, algebraic manipulations, leading ultimately to a description of the revised uncertainties with modifed correlations between the parameters. Figure 3.5 illustrates the revised uncertainties after calibration for the effective permeabilities of subdivisions of the BVG. (This Figure does not show the correlations between the parameters.) The revised uncertainties, including the correlations, were used in Probabilistic Safety Assessment calculations of the radiological risk from the repository.

4 Remarks

In this paper, the use of site characterization data in Nirex 97 has been outlined. The hydrogeological data can be divided into two categories: direct measurements of hydrogeological properties on various length scales, and measurements of derived properties. The former were used to derive an initial characterisation of the uncertainties in the effective hydrogeological parameters for regional-scale groundwater flow and transport models, and the latter were used to calibrate the models, leading to revised descriptions of the uncertainties. A key aspect of the analysis was the systematic treatment of uncertainties. The analysis enables the key uncertainties that impact on the risk to be assessed and traced back to their original sources. In the case of a continuing investigation programme, this provides a focus for possible future site characterization work. New techniques were developed to undertake the work, and advances in understanding were made.

Acknowledgment

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Figure 2.1 The initial uncertainties in the effective regional scale permeabilities for some of the hydrogeological units at Sellafield. The Figure shows the best estimate for a parameter (indicated by a diamond) and the estimated 95% confidence interval. Correlations between the parameters are not shown in this Figure.



Figure 3.1 Schematic illustration of the effect on the allowed region of parameter space of taking into account the constraints from calibration.





÷.

parameter

(b)







Figure 3.4 Example of the determination of a constraint from calibration (the environmental head for Nirex deep borehole 4). The calculated environmental head for the reference model is shown by the solid line and the calculated environmental head for variants with increased values of the parameter are shown by the lines with short dashes and the calculated environmental head for variants with decreased values of the parameter are shown by the lines with long dashes. Changes in lithology are indicated by the vertical band to the right of the plot.



Figure 3.5 Revised uncertainties after calibration for the effective permeabilities of subdivisions of the BVG. The Figure shows the best estimate for a parameter (indicated by a diamond) and the estimated 95% confidence interval. Correlations between the parameters are not shown in this Figure.

EVALUATION AND MODELLING OF A POTENTIAL REPOSITORY SITE - OLKILUOTO CASE STUDY

Pauli Saksa, Henry Ahokas
Fintact Ltd., Finland
Jari Löfman
Technical Research Center of Finland, Energy, Finland
Seppo Paulamäki
Geological Survey of Finland
Petteri Pitkänen
Technical Research Center of Finland, Communities and Infrastructure, Finland
Margit Snellman
Posiva Oy, Finland

Abstract

The observations, interpretations and estimates resulting from site investigations were developed into conceptual bedrock model of the Olkiluoto area. Model development has been an interdisciplinary process and three major iterations have occurred. Geochemical sampling and a programme of electromagnetic and electrical soundings were carried out and interpreted to model occurrences of groundwater types.

The parametrisation and modifications needed between geological models and groundwater flow simulation model is discussed. The latest groundwater flow modelling effort comprises the transient flow analysis taking into account the effects of density variations, the repository, post-glacial land uplift and global sea level rise. The main flow modeling result quantities (the amount, direction, velocity and routes as well as concentration of water) are used for evaluation of the investigation sites and of the preconditions for safe final disposal of spent nuclear fuel.

Integration of hydrological and hydrogeochemical methods and studies has provided the primary method for investigating the evolution. Testing of flow models with hydrogeochemical information is considered to improve the hydrogeological understanding of a site and increases confidence in conceptual hydrogeological models. Bedrock model allows also comparisons to be made between its time-varying versions. The evolution of fracture frequency, fracture zone structures and hydraulic conductivity has been studied. A prediction-outcome comparison was made in selected boreholes and showed that the rock type was the easiest parameter to predict.

1 Introduction

Posiva (formerly TVO) is carrying out site characterisation for disposal of spent fuel in the Finnish bedrock. At Olkiluoto field investigations has been in progress since 1980s. The first preliminary study phase lasted from 1987 to 1992 (abbreviated as SITU). Detailed site characterisation programme took place during 1993 - 96 (PATU). Now the work is under PARVI site evaluation phase (1997 -). Modelling activities of varying type have taken place during the years course some of which are discussed in this paper. The particular studies discussed and their position in time has been depicted in Figure 1.



Figure 1. Occurrence of modelling and evaluation studies discussed.

2 Modelling

2.1 Development of the geological model

The observations, interpretations and estimates resulting from site investigations have been developed into conceptual bedrock models of Olkiluoto area, located at south-west coast of Finland. The site area covers the western and central parts of the island. Geological models cover both lithology and structures. Model development has been an interdisciplinary process and several iterations have taken place. The bedrock model is compiled to Posiva's computer aided geological ROCK-CADTM modelling system (Saksa 1995).

The Olkiluoto site consists of Precambrian metasediments and plutonic rocks, 1850 -1900 million years in age. Migmatitic mica gneisses with cordierite and garnet porphyroblasts are the most abundant supracrustal rocks. They contain 20 to 50% neosome, which is most often granitic in composition. The mica gneisses are intruded by felsic plutonic rocks including oriented tonalites and granodiorites and massive, coarse-grained granites and pegmatites. The granites and pegmatites are very heterogeneous containing numerous mica gneiss restites.

The bedrock of the site records a polyphase deformational history. Five successive plastic deformational phases have been defined. The main deformation stage, D2, is a complex chain of events characterized by intense stratiform deformation with continuous production of neosome. During this phase the original bedding of the argilleous or sandy sediments was more or less destroyed, and foliation and metamorphic banding trending east-west were formed. Tonalite bodies were intruded into sediment layers. During the later deformation phases migmatites were folded by three subsequent folding phases. The main folding phase (D3) consists of NE trending folds with granitic veins and plastic faults parallel to the axial plane. After the plastic deformation phases the bedrock of the area began to respond to stress in a more brittle fashion resulting in scarp minor faults trending north and northwest.

First bedrock model was developed to cover interpretations and estimates of preliminary site investigations (in Fig. 1, version 1). It was based on surface studies and six core drilled boreholes. Both regional and site scales were covered. Modelling benefited from experience and observations of VLJ-repository volume.

Second modelling round took place during mid 1990s. New scanner type borehole logging tools were utilised in data collection. The bedrock model (version 2) contained data from eight boreholes, two investigation trenches and their interpretations. Lithological description was updated and more in detail. The knowledge of the lithological trend dipping between SE and SW was strengthened. The bedrock structure was described by 29 fracture zones four of which were completely new ones. Certain former interpretations had to be changed or abandoned. This was due to new seismic reflections observed. Properties or geometry was changed to 12 structures of the previous version of the model. Fracture zones were interpreted to be fairly conformant to lithology. Zone discrimination was based on expert judgment and statistical principal component analysis. Both interpretations and new observations indicated that fracture zones were likely to be more local and gently dipping than what was considered earlier.

The latest model revision took place in 1997 covering now 10 boreholes of the site. Observations lead to modification of four existing structures. One new fracture zone was introduced (version 3). Particular alternative conceptualisation has been formed to a unit comprised of two subhorisontal major zones (R17 and R20) as a whole.

Faulting can be a prominent structural phenomena within the bedrock volume studied. It might manifest itself in the form of difficulty to connect fracture zones from the surface to the boreholes and between the boreholes during interpretation. It has been suggested (Paulamäki & Paananen 1996) that the small scale faults parallel to NE trending D3 fold axis, can also be seen in site scale. One explanation to the discontinuous fracture zones could be, that the gently dipping fracture zones parallel to the foliation are cut and faulted by reactivated D3 fault zones, illustrated in Fig. 2. One of the interpreted fault

zones has been found in the investigation trench TK2 near borehole KR1 (Fig. 1). The trench demonstrated that the fault is a plastic one, but it has later been reactivated resulting in brecciated zone with calcite filled fractures. The subjothnian diabase dikes (age c. 1650 million years) found in the archipelago of southwestern Finland and the diabase of Olkiluoto are in this same direction indicating opening of fracture systems related to the intrusion of rapakivi magmas (Bergman 1986, Haapala & Rämö 1992).



Figure 2. Excerpt of the surface map of the Olkiluoto site bedrock model.

2.2 Groundwater salinity distribution and modelling

Previous drilling and related studies revealed saline groundwater, Total Dissolved Solids (TDS) over 35 g/l, below a depth of few hundred meters at Olkiluoto. From geochemical sampling, the origin of salinity was deduced to be partly from relictic seawater and partly from bedrock fluids. The knowledge of location of saline groundwater will serve as basis of evaluation of chemical corrosion risk, and providing starting values for numerical hydraulic flow modelling.

A model of bedrock groundwater salinity distribution was compiled. Starting point for model generation has been geophysical electromagnetic soundings (more than 350 in amount), that provided information on resistivity variations down to a depth of over one kilometer. Approximately 230 of the curves were interpreted using 1D layer model inversion. Observations from drilling, groundwater sampling, geophysical electrical (VES) survey and borehole logging, have been connected to the model and interrelated.

Obtained results have been gathered to ROCK-CAD system as TDS distribution model. The framework of the model is a set of undulating layers of downwards increasing salinity, Figure 3. Upper surface of saline water starts in the depth range 300 - 1000 m depending on the location. Varying weaker saline layers and bodies cover the upper part of the bedrock. In places, where weak mineral conductors do not disturb observation, a layer of brackish water has been found. A plume of fresh water, possibly controlled by fracture zones, has partly replaced saline water. TDS distribution model shows within depth 0 - 500 m also large spatial variations which are complex in form.



Figure 3. Cross section along holes KR2, KR4, KR6 and KR10 of the TDS model with the bedrock structures (version 2 model).

2.3 Groundwater flow modelling on the site scale

2.3.1 Conceptualisation

The objective of the modeling has been to provide results that characterize the groundwater flow conditions deep in the bedrock, and that can be used for evaluation of the investigation site and of the preconditions for safe disposal. The latest groundwater flow modeling effort of the site comprised the transient flow analysis taking into account density variations, the repository, post-glacial land uplift and global sea level rise. The analysis was performed by means of numerical simulation of coupled and transient groundwater flow and solute transport. The simulations were carried out until 10000 years after present. The basis for the numeric groundwater flow simulation has always been the most updated structural model. The model part was, however, complicated in its piecewise composition. Interference tests supported certain simplified and continuous structures in site scale and shown in Figure 4, for example, labeled as R19HY and R20HY. These structures together with nearly parallel structures R21, R17HY and R24HY explained almost all hydraulically active sections in different boreholes. Hydraulic conductivity in the rock mass is very low and strongly decreasing with depth.

The salinity of water samples may indicate that fresh surface water is infiltrating or migrating from recharge areas along some intersecting structures to deeper parts of the bedrock. This would happen especially within the central recharge area of the island. This evidence has supported the existence of some discrete hydraulic connections to be tested by numeric groundwater flow modelling.



Figure 4. Excerpt of surface map of the Olkiluoto site hydraulic-structural model.

Classification of fracture zones on ground of transmissivity was based on measured values. Structures without measured values were classified on the basis of geological significance. Measured transmissivities and two depth dependent curves for classification used are presented in Fig. 5. These gave the initial values of transmissivity for numerical simulations. In versions V1 and V2 (Fig. 1) structures were classified up to four classes and depth dependency of transmissivity (logT) was linear and stronger especially for deeper parts of the bedrock. It was estimated that linear extrapolation of transmissivities gave too low values especially for depths deeper than 1000 m. Numerical simulations indicated that values deeper than 1000 m are of minor importance. Reclassification simplified the structural model. Several minor structures with relatively low transmissivity were part of a larger structures or local in extent.



lg T (m²/s)

Figure 5. Measured transmissivities and two depth dependent curves for classification of structures for numerical simulations. Uncertain values depicted with open markers, crosses are values from VLJ-site studies. Range is given for certain structures by open circles.

In the hydrogeochemical field investigations at Olkiluoto salinity concentrations as high as 43 g/l (Cl) have been observed (Pitkänen et al. 1998). Variations in the density of water, caused primarily by the variations in the salinity of groundwater, have an effect on groundwater flow. The postglacial land uplift enlarges the area of the Olkiluoto island and raises the water table increasing flow of fresh water deeper into the bedrock and a mixing of water of different types. Because the remaining uplift is still expected to be several tens of meters (Eronen et al. 1995, Påsse 1997), the flow conditions at Olkiluoto are slowly evolving causing ongoing changes in the hydrology of the area. Because of the varying salt content of groundwater and the effects of the land uplift, the flow analysis called for coupled and transient modelling of flow and solute transport. The analysis was performed from the present until 10000 years after present (A.P.), when the next ice age is assumed to occur.

The fractured bedrock was modelled employing a concept of hydraulic units: the twodimensional, planar shaped fracture zones and the remaining part of the bedrock (intact rock). Within each hydraulic unit the equivalent-continuum (EC) approach was applied, i.e. each fracture zone and intact rock were separately treated as a homogeneous and isotropic continuum with average characteristics. The repository was modelled as a twodimensional object.

2.3.2 Flow and transport model for the Olkiluoto site - Results

The modelled volume was disretized into finite element mesh containing three-dimensional hexaedral elements representing the intact rock embedded with two-dimensional quadrilateral and triangular elements for the fracture zones. The location and size of the repository were based on the repository layouts (Saanio 1997). The present groundwater table (Saksa et al. 1993) together with a mathematical model describing the land in the Olkiluoto area (Påsse 1997) were employed as a boundary condition at the surface of the model, while the initial and boundary conditions in the rest of the modeled volume were based directly on the measured salinity concentrations along the cored boreholes (Pitkänen et al 1998). TDS distribution model supported the geometry of salinity chosen to numerical simulations.



Figure 6. Computed TDS concentration at vertical south-north cross-section (same as in Fig. 3) of the modelled volume.

The result quantities were the amount, direction, velocity and routes as well as concentration of water, which were considered especially in vicinity of the repository. A major part of water flows into (out of) the repository from above (downwards) along the intersecting fracture zones R10HY and R16, and through the rock matrix. Situation is illustrated by Figure 7. The amount of water flowing through the repository increases with time as a result of land uplift and fresh water intrusion. The most important flow routes from the repository to the surface are along the fracture zone R21, which dips from the north-west below the repository, and along the zone R27, which is directed to west (Figures 3 and 7). The results computed with and without the repository showed that it has only a small effect on the flow conditions. The salinity of groundwater in the bedrock decreases with time, and at 10000 years after present there is practically only fresh water at the depth of repository (500 m) (Fig. 6).



Figure 7. The dominant flow paths from the repository.

2.4 Hydrogeochemical assessment and implications to flow modelling

Integration of hydrogeological and hydrogeochemical methods and studies provides the primary tool for investigating the evolution in the past, and for predicting future conditions. In addition hydrogeochemical information has been used to screen relevant external processes and variables for definition of the initial and boundary conditions in hydrological simulations.

Hydrogeochemistry shows that the groundwater at the Olkiluoto site is a mixture of at least five end-member water types (Table 2-1) derived during paleohydrogeological and modern processes (Pitkänen et al. 1996). Fresh, diluted groundwater is confined to shallow depths. Brackish Na-Cl type water occurs at depths of 100 - 500 m, and salinities as high as 70 000 mg/l has been observed in deep-occurring saline Ca-Na-Cl type groundwater.

Brackish Na-Cl groundwater enriched with SO_4 has been identified at a depths of 100 - 300 m. The salinity of this water type clearly exceeds the present value of the Gulf of Bothnia (Cl \approx 3 600 mg/l), while the Br/Cl and stable isotope ratios of water are similar to that of sea water. Below this SO₄-rich layer of brackish groundwater the level of heavy stable isotopes falls, reflecting the mixing with colder climate water. At greater depths, the stable isotopic composition of saline groundwater (Cl_{max} 43 000 mg/l) tend to shift above the global meteoric water line. The Br/Cl ratio of this water also rises significantly above the value for sea water.

At Olkiluoto fresh, meteoric groundwater has been infiltrating since the land rose above the sea level 2500 years ago. According to the hydrochemical and isotopic characteristics of the SO_4 -rich brackish groundwater, it is most likely that the infiltration has come from the Litorina Sea. The depletion of heavy stable isotopes can be explained by mixing with colder pre-Litorina water, probably meltwater from the Weichselian ice sheet. The chemistry implies that the displacement of meltwater by denser Litorina water decreases in the brackish groundwater below the SO_4 -rich layer and, in addition the proportion of the saline end-member gradually increases. The deep location below the cold endmember and elevated stable isotopes are indicative of a pre-glacial origin for the saline water. Hydrogeochemical characteristics are assumed to reflect hydrothermal conditions (Blyth et al. 1998) and an early pre-Quaternary origin for the saline end-member according to the known geological history of the Fennoscandian Shield (Pitkänen et al. 1996).

Depth of	Water-type	Origin of dominant end-	Age estimate of
occurrence		members	main end-members
<150 m	Fresh-slightly	Meteoric water and	0 - 2 500 BP
	brackish HCO3 -	modern Baltic water	
100-300 m	SO ₄ -rich brackish	Litorina Sea water	2 500 - 7 500 BP
	Na-Cl water		
100-500 m	Brackish-saline	Pre-Litorina water with	10 000 BP
	Na-Cl water	fresh glacial meltwater	
>500 m	Saline Ca-Na-Cl	Preglacial water influenced	>> 10 000 BP
	water	by hydrothermal brines	

Table 2-1.Main water-types at Olkiluoto and predicted age of dominant end-member-types (Pitkänen et al. 1996).

3 Evaluation of the model

3.1 Testing of previous results and assumptions

One of the topics of the characterisation programme 1993 - 96 was the testing of the site knowledge and previous results. The subjects considered were rock type, fracture density, occurrence of fracture zones and hydraulic conductivity of the intact rock. Each subject had an established claim in the background - like "regional rock types are prevailing within the site volume" - which was tested. Results from the earlier work phases were compared with the latest data available and the trend was studied.

For Olkiluoto the outcome of the testing was:

- the main rock types (gneisses, granite/pegmatites and tonalite) are dominating by all measures.

distributions of the fracture densities are similar, no statistically significant differences existed. This applied both to the surface 0 - 300 m and to deeper > 300 m bedrock part.
fracture zones have occupied earlier 12.8 % of the total borehole length. This has reduced to 9.4 %. The average intersection length has lowered from 10.4 m to 9.2 m. The number of interpreted fracture zones has accompanied the increase of borehole meters. New investigation methods have increased the knowledge level somewhat - model structures explained during 1992 64.1 % of borehole sections and during 1996 68.8 %.
statistics of the hydraulic conductivity values were the same in the depth range 0 - 300 m for the both investigation phases. Data for deeper bedrock shows slight increase for conductivity values.

3.2 Prediction-outcome tests for the borehole data

Also a prediction-outcome comparison tests were made in boreholes KR2 extended part and in borehole KR10. Lithology prediction diverged (statistically) from the observations but only a few percents of the rock was of accessory type. Predictions for the fracturing overestimated the fracture density. This is partly due to the assumption that the rock within the fracture zones would be densely fractured throughout which not seemed to be the case. Hydraulic conductivity estimates gave lower and higher values than what was measured in the holes. More than 90 % of the observed hydraulic conductivities were within estimated 90 % confidence limits.

3.3 Other evaluation activities

Recent pumping tests (spring -98) have strengthened the existence of the most dominant fracture zone R20HY - e.g. strong pressure responses deep in the borehole KR9 at a distance of almost 500 m. On the basis of long-term pumping test and flowmeter measurements it was found too that the very high transmissivity value measured with double packer injection test at depth of 310 m (see Fig. 5) is a local phenomena i.e. the transmissivity (log) of structure R20HY in the borehole KR4 is about -4.5 instead of having value of -3 given in Figure 5.

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SCIENCE DESIGN FOR TWO SHAFTS IN PHASE 1A OF THE PROPOSED ROCK CHARACTERISATION FACILITY AT SELLAFIELD, UK

Peter Ledingham, GeoScience Ltd, Falmouth, UK Anthony J. Proughten, GIBB Ltd, Reading, UK George J. Saulnier Jr., Duke Engineering & Services, Austin, Texas, USA

Abstract

In 1997, United Kingdom Nirex planned to begin construction of an underground Rock Characterisation Facility (RCF) at Sellafield as part of it's ongoing assessment of the suitability of the site as a host for a deep radioactive waste repository. The RCF was to have addressed issues relating to the geology, hydrogeology and geomechanical behaviour of the site by collecting data for testing predictive models and acquiring information only available from an underground situation.

In March 1997, the UK Government refused permission for Nirex to begin construction and work at Sellafield was wound down. However, the science design for Phase 1a of the RCF, two vertical access shafts, was completed to provide a set of conceptual designs which address the issues identified by Nirex. By using Sellafield as an example, the designs contribute to a series of reports which demonstrate an approach to validation using an underground facility.

This paper describes the Science Design for data collection during shaft construction, which began with the information requirements specified by Nirex on the basis of it's conceptual models and predictive work. It describes the scientific measurements designed to acquire this information and the process of combining the individual measurements into test plans for each shaft.

Measurements were planned in the shafts themselves and in boreholes drilled from the shafts. They were designed to provide data on formation porosity and permeability, the geochemistry of formation water and the nature of the fresh-water salt-water interface, shaft inflow, the influence of geological structures on performance, and geomechanical responses to shaft excavation.

A key element of the design process was the development of test plans, requiring the coordination and integration of the construction and science activities so that both could be carried out in a timely and cost-effective manner.

1 Background

In 1994 United Kingdom Nirex Limited (Nirex), as part of an extensive programme of scientific investigations to determine whether or not the site was suitable for construction of a deep repository for the disposal of intermediate-level radioactive wastes, applied for permission to construct an underground Rock Characterisation Facility (RCF) near Sellafield in west Cumbria, UK.

The application followed an extensive surface-based site investigation during which 29 deep boreholes were drilled and tested to investigate and develop a three-dimensional understanding of the geology and hydrogeology of the subsurface formations in the area. The scientific programme planned for the RCF was designed to follow on from this work and run in parallel with an ongoing surface-based investigation, the Nirex research programme and safety assessment studies.

Assessments of the safety of a potential repository in 1995 identified a number of key issues which needed to be addressed in the RCF before Nirex could have taken a decision on whether to propose a repository at the site. These issues related to aspects of:

- groundwater flow and radionuclide transport;
- the natural and induced changes to the geological barrier; and
- the design and construction of the repository.

These issues were to be addressed in the RCF by collection of data with which to test the predictive models of the site behaviour, with respect to geology, hydrogeology and geomechanics.

2 The Sellafield RCF

The planned RCF was to have comprised a series of horizontal galleries at a depth of approximately 700m, giving access to a reasonably large portion of the potential repository zone and providing sufficient space to carry out experiments in isolation from one another. The galleries were to be accessed by two vertical shafts (the North and South Shafts) in the centre of the facility and separated by approximately 50m.

Construction of the RCF was to have taken place in three phases over about 10 years. Phase 1 was the sinking of the two shafts and their connection by roadways, Phase 2 was construction of galleries within 200m of the shafts, and Phase 3 was extension of these galleries to a total length of 975m. Phase 1 was further subdivided, with Phase 1a being sinking of the shafts alone (i.e no connecting roadway). The Science Design described in this paper applies to Phase 1a.

The two shafts were to be concrete lined through the sedimentary rocks but unlined in the potential host formation, the Borrowdale Volcanic Group, with a finished diameter of 5m.

In recognition of the geological formations to be encountered, the likely construction methods required and the scientific objectives, the shafts were divided into 11 Sectors; Nos. 1 to 7 in the South Shaft and Nos. 8 to 11 in the North Shaft. Sinking of the North Shaft was planned to lag behind that of the South Shaft in terms of depth and the phasing arranged so that inter-shaft testing could be carried out. The planned duration of Phase 1a was approximately 3 years.

3 Information requirements

Two kinds of scientific information were required; data which could only be gained from underground investigations and data to test gross and Sector-specific models of the geology, hydrogeology and geomechanics of the site.

The data only available from underground investigations included specific data requirements for Phase 1a, in particular the nature of fractures and their variability over length scales greater than that available from boreholes, the characteristics of flowing fractures, stress-dependent behaviour of the flow system, the response of the rock mass to the excavation process and certain hydrochemical data.

Thirty-five models were identified for testing during Phase 1a, at a number of scales from local to regional. Eight of the models were geological, four of which were deterministic and four probabilistic to describe spatially variable properties such as structural domains and sedimentary architecture. Eighteen hydrogeological models were developed, using the geological models as a framework. In addition to the normal hydrogeological parameters, these models also included hydrochemical models of the variations of groundwater chemistry within the potential repository zone. Nine geomechanical models were developed to assess the mechanical behaviour of the rock mass during and after construction, four of which were simple hydromechanical models to assess coupled behaviour of discontinuities close to the shafts.

These information requirements were translated into a schedule of measurements to be undertaken during shaft sinking and formed the basis of the Science Design. From this schedule and outline test plans, a series of individual measurement designs and detailed integrated test plans was developed. The measurements, their distribution and key design features are summarised in Table 3-1 and described in the following sections.

4 Geological Measurements

The design for the principal geological measurement, *Geological Mapping*, consisted of the observation and recording of geological, geomechanical, and hydrogeological features seen in the underground excavations, and the sampling of geological materials. Mapping requirements, in terms of type of feature and amount of detail to be recorded, would vary throughout the excavations. A mapping method was required to ensure that no geological features of possible significance would go unnoticed and unrecorded by mappers. The recommended method allowed for high resolution photographic images of all excavated surfaces to be made, together with inspection of all newly excavated faces

which would allow decisions to be made about which geological features should be subsequently recorded by the mappers onto previously prepared hard copy photographic images.

A principal feature of the mapping design was the imaging system. The shaft wall was to be imaged around its circumference with a rigidly mounted digital camera. The camera would be rotated between exposures to give a series of consecutive frames, with horizontal and vertical overlaps of 50% and 10% respectively. This technique provides 'high resolution' images that are at least as 'sharp' as high quality photographs and capable of being enlarged, like photographs, without losing sharpness of relevant detail. In addition, digital images would be stored electronically in the project database. A number of imaging systems were reviewed, and a system was recommended for further investigation. Because potentially significant developments are being made in digital imaging systems, the final choice of system would be made as late as possible in any final design process.

An additional design requirement was that the shaft wall was to be profiled after every blast round. The number of profiles and density of measurements within each profile were designed to vary according to the level of detail of geological information recorded. The design recommended a commercially available downhole scanner, comprising a computer-controlled automatic scanning laser profiler, designed to profile underground cavities.

The mapping process would be undertaken within each shaft sinking cycle and would commence with the Mapping Team being called out and then travelling to the science deck of the sinking stage with their equipment. Digital images would be acquired from beneath the science deck, followed by a profile of the shaft walls. While imaging and profiling was taking place, mappers on the science deck would record geological information on mapping forms and on a mapping template consisting of an image of the shaft walls made during a previous mapping shift. The mappers would take samples as necessary (using a barcode labelling system for sample tracking and control) and then return to surface where they input all the information they have collected into the database.

Core Logging procedures were prepared based upon those developed for the previous surface-based acquisition programme. It was proposed that *Core Orientation* should be carried out by correlation of borehole wall imagery with discontinuities in the core. A slimhole imaging system was proposed comprising an optical logging tool supported by a workstation for derivation of discontinuity orientations. Visual correlations would then be made between specific discontinuities clearly identified in the core and on the imagery. Sticks of core would be oriented using several correlated discontinuities per stick, and apparent discontinuity orientations recorded during core logging would be corrected.

5 Geomechanical Measurements

Selection of the shaft spacing was based on engineering considerations, but was also intended to preclude significant interaction between the stress-strain fields developed around each shaft in response to excavation. Furthermore, the South Shaft was to be sunk in advance of the North Shaft, resulting in both spatial and temporal separations between the excavation-induced responses of the rock mass around each shaft. These responses would have resulted in the development of excavation disturbance zones (EDZs) around each shaft, in which the mechanical and hydraulic properties of the rock mass are expected to change.

The design of the *Response to Excavation* measurement comprised the drilling and instrumenting of boreholes from the North Shaft and the South Shaft, in advance of the North Shaft, into a block of ground through which the North Shaft would later pass. The key design issues for these measurements were therefore; optimisation of the location of instruments with respect to the anticipated *EDZ*; simplification of installations to minimise the risk of instrument failure (i.e. limit multi-instrument installations in single boreholes); and the minimisation of disruption to shaft-sinking operations and programme by planning activities to avoid the programme critical path.

At each measurement location, changes in the selected parameters were to be measured in a plane perpendicular to the axis of the North Shaft. It was assumed that the distribution of excavation-induced changes would be anisotropic but axisymmetric (i.e. with respect to the axis of the North Shaft). Instrument array layouts targeted the specified plane or horizon and, as far as practicable, all instruments were to be installed in this plane. The preferred arrangement of boreholes and instruments consisted of:

- an array of three overcoring stress measurement, stress-change monitoring and *acoustic emission (AE) monitoring* boreholes drilled from the North Shaft. These to be inclined at -70°, separated by 120° intervals in azimuth. This layout was determined in part by the geometrical requirements of the AE system, and by the need for the strain monitoring cells to be within the North Shaft EDZ.
- an array of three extensometer & packer extensometer boreholes drilled from the South Shaft in advance of North Shaft excavation at a nominal inclination of -5°.

Each borehole was to be geologically and geophysically logged to assist in the identification of features of interest. Cross-hole *seismic tomography* carried out between boreholes drilled from the South Shaft would provide data to assist locating individual instruments. Short, sub-horizontal boreholes drilled from the North Shaft at each of the three locations, would allow measurements for *estimation of mechanical rock properties* conducted using a specifically-developed proprietary ultrasonic logging tool. The overcoring stress measurements were to be carried out using CSIRO HI cells, and would provide information on the undisturbed stress tensor prior to excavation of the North Shaft in the zone of interest. On completion of overcoring stress measurements, CSIRO HI cells would be installed to monitor stress changes in response to excavation.

The *acoustic emission monitoring* system design allowed for two sets of sondes. The first (termed the AE system) was designed to monitor high frequency events (around 50 kHz) in the near-field, associated with excavation-induced rock fracturing. These sondes were also capable of transmitting signals to allow seismic interferometry to be conducted in the zone of interest. The second set of sondes (the microseismic or MS system) was designed to monitor lower frequency events (less than 10 kHz) in the near and far-field, associated with redistribution of the *In situ* stress field. Detailed procedures for active AE testing and passive monitoring were developed to allow the development of the EDZ to be assessed during the excavation of the North Shaft through the zones of interest. This involved a quiet period of four hours when sources of external acoustic and electrical noise were to be minimised. The AE system would be removable, whilst the MS system would be left in place for long-term monitoring.

The array of boreholes drilled from the South Shaft consisted of two Borehole Fracture Extensometers (BOF-EXs) and one Packer Extensometer (PAC-EX). The BOF-EXs were to measure strain in the specified plane around the North Shaft, and provide a continuous profile of measurements from the most disturbed areas close to the shaft wall, to essentially undisturbed conditions remote from the shaft. Measurements were to be made in a zone extending from approximately 0.5 to 3 diameters from the shaft.

Because of their arrangement in plan, BOF-EX measurements would include components of both radial and tangential strains which it would not be possible to separate. The measurements were designed in two adjacent quadrants to provide information on strain and stress anisotropy. PAC-EX instruments were to be used to monitor changes in the mechanical aperture of selected fractures as a function of time, hydraulic pressure and radial distance from the North Shaft. Active testing of the instruments could also be carried out and would involve perturbing the system by increasing or decreasing pressure in the test zones, and monitoring displacements, pressure changes and pressure-recovery times.

6 Hydrogeological Measurements

The hydrogeological measurements were designed to determine the *In situ* hydrogeological conditions in the formations penetrated by the shafts and to estimate shaft impact on local hydrogeology. Specifically, the measurements included:

- Quantification of the inflows of groundwater into the shafts during construction;
- Measurement of near-field, and possibly far-field, formation fluid pressures in boreholes drilled from the shafts;
- Collection of groundwater samples for hydrochemical analyses and installation of instrumentation for the *In situ* measurement of Eh, pH, temperature, and chloride;
- Formation hydraulic testing in probe holes in advance of excavation;
- Formation hydraulic testing in boreholes drilled from the shafts; and
- A long-term pumping test to explore the impact of the shaft construction on the Brockram formation, immediately above the potential repository formation.

Inflows of Groundwater into the Shafts were to be quantified by measuring the inflow and outflow from the shafts and calculating the net groundwater flux. The shafts would have acted as large diameter well(s) for at least part of the construction period and their hydrogeologic impact was to be estimated from the quantities of groundwater flowing into them. The design provided a detailed methodology for flow monitoring of construction water, estimating the inflow from singular hydrogeologic features, and monitoring the water pumped from the shaft sump. The basic monitoring would calculate the net flux to or from the shafts from the construction water, water pumped from the shaft, and the fluid drained from the shaft muck, all recorded daily on the science programme's Automated Data Acquisition System (ADAS). Water garlands installed on the shaft wall below zones of enhanced drainage would provide an additional means to observe the inflow capacity of the formations penetrated by the shafts.

The construction water was also to be tagged with tracers to provide a quantitative estimate of the amount of construction fluid returned to the surface. The tracers would be a mixture of a colorimetric tracer, sodium fluorescein, and a conservative organic tracer, benzoic acid. Sodium fluorescein would provide a field determination of the constructionwater dilution which would be confirmed by HPLC analysis of the benzoic acid.

The design for *Groundwater Pressure* measurement allowed for the collection of data with which to estimate the long-term fluid-pressure response of the local formations during and after construction. After construction, the formation fluid pressure of formations sealed by the shaft lining would recover while those in the unlined portion of the shafts would depressurise to a steady condition. Groundwater pressures would be observed using single and multiple-packer configurations and long-term monitoring instruments. Boreholes would be set in recesses in the shaft wall to allow for long-term maintenance.

Hydrochemistry of the groundwater in formations penetrated by the shafts was to be determined by collecting and analysing water samples from boreholes and shaft inflows, and from *In situ* hydrochemical monitoring equipment installed in sealed boreholes drilled from the shafts. Analysis would include species sensitive to oxidation state and atmospheric contamination such as Fe species, Eh, pH, alkalinity, ¹⁴C, helium, and dissolved gases. The *In situ* equipment package would have comprised instruments, packers, valves and flow cells. The potential contamination of samples would be evaluated by monitoring tracer concentrations using field fluorometry to determine sampling time. Only groundwater samples with less than 1% tracer concentrations would be based on analysis of benzoic acid tracer concentrations.

Probe-Hole Hydraulic Testing of sequences of up to four probe holes drilled before each segment of shaft excavation was to be used to establish the pressure and flow potential of formation-fluids below the current location. A testing sequence was developed to measure cumulative flow from the probe holes; determine the probe hole with the largest volume of flow; identify significant hydraulic connections among the probe holes, and collect groundwater samples for field and laboratory analysis. Probe-hole testing equipment would comprise a single expandable packer to divert flow and isolate the probe holes so as to more fully characterise singular hydrogeological features, rather than the entire length of the probe hole.

Hydraulic Testing in Boreholes drilled from the shafts at selected depths were intended to provide estimates of the bulk hydrogeological parameters for the formation, to provide fluid-logging profiles of the distribution of inflow or outflow along the length of boreholes, and to provide pressure versus time data for selected isolated zones. Crosshole testing would be used where possible, to examine the rocks around the shafts and between the boreholes. Testing would comprise sequences of flow and shut-in periods, usually initiated by shutting in boreholes as soon after drilling and geophysical logging as possible to monitor pressure recovery data. The total-flow and pressure-recovery data would be used to estimate bulk-transmissivity, and provide formation-to-formation and borehole-to-borehole comparisons. Full profile evaluation would be obtained using "moving packer" fluid-flow logging to observe salinity contrasts in low-permeability formations.

Boreholes used for testing would also be used for long-term fluid-pressure monitoring, so shaft wall recesses for borehole wellheads were created to allow the installations to be protected from excavation and post-construction activities.

All hydraulic testing would be monitored and controlled with a portable data acquisition system using the real-time data-analysis software GTFM to optimise testing time, account for pre-test borehole-pressure history, optimise estimates of formation parameters, and provide estimates of the confidence in estimated parameters. Active tests would be terminated as soon as performance objectives are met, or if further improvements in confidence levels were not possible.

Long-Term Hydraulic Testing of the Brockram Formation, a key formation above the potential repository host rock, was designed to evaluate the long-term effects of the shafts and determine whether a pressure signal could penetrate into the host rock. One or more boreholes would be drilled from the base of the South Shaft and tested using a constant-pressure production method with an imposed sinusoidal variation in rate or pressure to uniquely identify the test's pressure response.

Responses would be monitored in the site-wide network of boreholes with multi-packer systems to evaluate regional permeability anisotropy, along with tracer additions. The production borehole would be equipped with a high-pressure control valve, a digital flow meter, a sampling port, a pressure controller to control flow rate variations, all monitored with a smart data acquisition system. The long-term test would be optimised using GTFM real-time analysis software.

7 Integration with construction

The design of the RCF comprised two elements; the engineering construction of the shafts and the scientific programme, which were to be carried out concurrently. These two elements required careful integration both to ensure that the scientific objectives were not compromised by the construction activities and that the construction activities were not unreasonably impacted by the science programme.

In addition to developing individual measurement designs, detailed Sector Test Plans were drawn up showing the locations and interactions of the measurements. These plans demonstrated how the required data collection would be acquired in a cost-effective manner, with the lowest disruption to shaft construction operations, and were a major element in the overall design. Mutual early planning also allowed the Shaft Sinking Contractor to plan scheduled activities, work schedules and crew changes, equipment maintenance and changeover, and safety activities. Regular collaboration meetings were held to anticipate and identify potential activity conflicts and establish working solutions.

Particular problems addressed in this integration process were the timing of tests, working space constraints, protection of equipment from blast damage, sequencing of test installations in sections which had to be lined, management of water inflows, safety and co-operation in the provision of services. Some tasks were duplicated in the construction and science designs and the responsibilities were optimised at this stage.

Scheduled monitoring of construction data jointly managed by the Science and Shaft-Sinking Contractors was also planned, with the objective of ensuring collection and preservation of data relevant to the science activities and their interpretation.

8 Data Management

Data Management procedures were developed in the form of a comprehensive Information Management System (IMS) to ensure that all construction, monitoring, and testing information would be properly collected, archived, and made available for retrieval. This information would consist of either electronically or manually recorded data uniquely identified along with it's relationship to other information.

Linkage of the IMS data streams would ensure that the large number of interactive science tests could be tracked accurately and allow real-time decision making regarding test durations and modifications whilst maintaining scientific integrity. The data-collection function was designed for user access and to be flexible enough to allow corrections as needed. The IMS would also have available information such as calibration data to assure data quality.

The science database would be linked to a graphics-and-analysis package to allow data display in multiple graphical formats and performance of basic filtering using specialised data-analysis software including compatible data/software formats.

Information retrieval would be via a graphical user interface allowing a multiplicity of formats to meet the needs of the users, with specific criteria for time, location, type of information, and relationship to other information in the database. The database would operate as a satellite to the Nirex RCF Database, which was to have been the central repository for both construction and science-related information. The IMS would also have been linked to and integrated with the pre-existing site-wide historical database.

9 Summary

The testing plans developed in the science design for the shaft-construction phase of the proposed RCF represented an effort to obtain a body of data to provide a baseline, early-time representation of hydrogeological conditions and geomechanical integrity of the rock mass around and above the RCF before it was fully constructed. The Science Programme was designed interactively with Nirex and the Shaft-Sinking Contractor to ensure timely and cost-efficient data collection without compromising either scientific objectives or construction quality.

Because the state of stress, the hydrodynamic equilibrium, and the local hydrochemistry would change in the months and years following construction, data collected during the construction period would be an important benchmark against which all future changes can be compared.

The Science Design incorporates state-of-the-art technologies such as digital imaging, *In situ* hydrochemical and geomechanical instruments, acoustic emission monitoring techniques, benzoic-acid tracers and real-time test-analysis software. A high-capacity, interactive data-acquisition system was planned as part of a comprehensive data-management system, designed to assure data integrity and accessibility within a defensible Quality-Assurance framework.

10 Acknowledgements

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Finally, we thank Nirex for permission to publish this paper.

Table 3-1 Summary of measurements included in the Science Design

Measurement	Purpose	Frequency / Location	Key Design Elements
M1 - Geological mapping	Geological mapping & imaging of shafts, to provide information for correlation with data from other Measurements.	Routine; after every blast round. Specialist; at predetermined targets and zones of interest.	Digital imaging with data mapped directly onto hardcopy. Shaft profile at 1m depth intervals and 5° angular increments.
M2 - Inflows of groundwater	Identification of all inflows, water balance, and calculation of net groundwater inflow.	Continuous measurement of traced construction water into shaft and pumped water out of shaft. Daily water balance.	Measurement and tracing of construction water. Water garlands and bird's nests to capture water at shaft wall. Stage-pump to surface. Measurement of all flows.
M3 - Groundwater pressures	Continuous monitoring of groundwater pressures in boreholes from the shaft walls to determine post-construction pressure recovery.	Continuous long-term measurement of pressure in all borcholes drilled from shafts for testing, sampling, and geomechanical testing.	Single and multiple packers with pressure transmitters to monitor pressures. Sealing standpipe recessed into shaft wall. Data integrated with site-wide database.
M5 - Hydrochemistry	Sampling and monitoring of representative groundwater from formations penetrated by the shafts.	Boreholes at least once per formation and at regular spacing through saline transition zone. Long-term <i>m situ</i> monitoring of hydrochemistry.	Sampling as soon as possible after drilling. Field analysis of tracers to qualify water for laboratory analysis. Probes installed <i>in situ</i> to monitor Eh, pH, Temp., and chloride.
M6 - Drilling	Provision of borcholes, usually cored, for subsequent in situ testing and monitoring.	As required by other Measurements.	Small stage-mounted rig for short shaft wall boreholes. Computer-controlled, modular longhole rigs for drilling from shaft floor. Barcoding system for control of core.
M7a - Geophysical wireline logging	Geophysical logging data in support of other measurements.	In cored and uncored borcholes drilled for other Measurements, as required.	Slimhole tools. Density, sonic, resistivity, porosity & gamma logs required.
M7b - Core orientation	Core orientations to determine the 3D spatial co-ordinates and orientations of discontinuities.	In cored boreholes drilled for other Measurements, as required.	Borehole optical imagery system to determine discontinuity orientations. Discontinuity logging procedures include corrections using imagery data.
M8 - Hydraulic testing in probe holes	Simple flow monitoring, pressure recovery and hydraulic testing in probe holes drilled in advance of the shaft.	Probe holes drilled every 30 metres during shaft sinking. Routine testing in every set, specialist testing in each formation.	Sequential boreholes to allow monitoring during drilling. Portable data acquisition system to observe testing at the sump level. Use of square-wave hydraulic tests to isolate test from other influences.

Table 3-1 continued....

Measurement	Purpose	Frequency / Location	Key Design Elements
M9 - Hydraulic testing in boreholes	Hydraulic testing in borcholes drilled from shafts into specific targets.	Boreholes in each formation and into specific geologic targets.	Obtain total flow. Use moving packer or fluid- conductivity sonde for flow logging. Real-time test analysis to optimise testing.
M10 - Pumping test in the Brockram	Long term pumping test to characterise the Brockram formation.	Long boreholes drilled from North Head Member into Brockram. One test only.	Use packer and electronic flow control. Constant-pressure test with an imposed sinusoidal signal to identify test response. Real-time analysis to optimise testing.
M11 - Collection of rock samples	Sampling of rock materials in the shafts for examination and testing.	Concurrent with routine mapping and from key target areas underground.	Barcode-based system developed to provide sampling and testing history. Collection from muckpiles in shaft and at surface.
M13 - Response to excavation	Quantification of the geomechanical response of the rock mass to excavation of the shafts.	At specific locations (lithologic units) in the shafts. Three tests only, plus triaxial strain measurements in the Sandstone units.	Measurement of in situ stress (overcoring), displacement across natural fractures (MPBXs), changes in hydraulic properties of fractures (packer-extensometers), and triaxial strain monitoring. Integration of data with core, wireline logging, hydraulic testing, material properties, tomography and acoustic emission test data.
M14 - Mechanical properties estimates	Estimate Young's modulus (E), rock mass modulus (G) and Poisson's Ratio of rock adjacent to shaft walls.	Within specific lithologic units, and to correlate with M13 locations.	Seismic compressional and shear wave velocities measured using a proprietary ultrasonic logging tool.
M16 - Tomography surveys	Crosshole seismic tomography data to provide information on rock mass structure.	Within specific lithologic units, and to correlate with M13 locations.	P-wave: Spark discharge source and multi- element hydrophone string. S-wave: Borehole hammer source and clamped multi-element receiver string.
M17 - Acoustic emission monitoring	Monitoring of seismic activity induced by shaft excavation as part of M13.	At the same locations as M13.	High frequency (AE) to detect near-field activity and lower frequency microseismic monitoring system to detect near & far-field events. AE sondes can also be used for seismic interferometry.
M19 - Monitoring construction data	Ensure that construction data of use to science program is routinely collected.	Daily monitoring of all relevant data. Enter data into site-wide database.	Co-ordination of data collection to minimise interference with shaft-sinking operations. Use of dyes to track cement grout paths.

PLANNING FOR INVESTIGATION AND EVALUATION OF POTENTIAL REPOSITORY SITES IN SWEDEN

Karl-Erik Almén, KEA GEO-Konsult Anders Ström, SKB

Abstract

The present stage of siting of the Swedish Deep Repository for spent nuclear fuel involves general siting studies on national and regional scales and feasibility studies on a municipal scale.

Based on these studies, two areas will be selected for surface-based site investigations. The geoscientific site information will be used in the site evaluation process, in which performance and safety assessments and design studies are the major activities, in combination with geoscientific characterization. The safety report and EIA document from the site investigation stage will be the most important documents in the application for the siting permit and the permit to construct the deep repository. Detailed characterization (including tunnels and shafts down to repository level) will then verify the suitability of the selected site.

The programme for geoscientific site investigations is based on experience from more than 20 years of field studies in several SKB projects, such as the Study Site Investigations, the Stripa Project, and the Äspö Hard Rock Laboratory. The strategies and methodologies developed, implemented and verified within the Äspö HRL are a very important source of information and know-how for the development of the site investigation programme.

The investigations will produce geoscientific models that include all information needed to analyze the long-term safety of a deep repository located in and adapted to the geological conditions of the rock. The type of geoscientific information needed for performance and safety assessment, layout and design, environmental studies and for fundamental geoscientific understanding has been specified and compiled in a "parameter" report.

The general strategy is that performance assessment, layout and design studies will be conducted in parallel with the geoscientific investigations. Information will be transferred at logical occasions, when decisions have to be taken and when feedback is desirable for new investigation steps. The role of the geoscientific evaluation is to act as an engine for this information exchange between the different activities.

1 Introduction

1.1 Background

The Swedish system for nuclear waste management involves an excavated repository for spent nuclear fuel at a depth of about 500 m in crystalline rock, see Figure 1. The spent fuel will be encapsulated in steel/copper canisters, which will be placed in deposition holes drilled in a system of tunnels. Blocks of swelling bentonite clay will surround the canisters in the holes. Upon sealing of the repository the tunnel galleries will be backfilled with a mixture of crushed sand and bentonite. The disposal concept is a result of an extensive research programme conducted by SKB since 1977. The most important geoscientific investigations for describing rock properties at repository depth and for understanding the behaviour of groundwater flow and chemistry in the rock have been:

- the study site investigations, conducted 1977-1986, in which several sites with different types of rock were characterized,
- the Stripa project, conducted 1977-1992, which involved research on rock properties and development of characterization methods,
- the Äspö Hard Rock Laboratory, started in 1986 and still in progress, of which the first phases (pre-investigation and construction) involved a systematic characterization and evaluation programme aimed at verifying pre-investigation methodology.

Long-term performance and safety studies (based on generic as well as on site-specific data), design and rock engineering studies and comprehensive research on the geoscientific processes of importance for repository function are other components of the technical preparations for the deep repository (SKB 1995, a).



Figure 1 Conceptual repository design.

1.2 General outline of preparations for the deep repository

The general outline of the process of establishing the deep repository involves:

- siting studies
- site investigations
- detailed characterization (including partial repository construction)
- repository construction and repository operation

The siting studies involve the following activities:

- general siting study of the whole country; reported in 1995 (SKB 1995, b),
- general siting studies in counties; ongoing,
- feasibility studies in municipalities; two reported and three ongoing.

The general goal of the siting activities is to prepare for the selection of candidate areas in two municipalities, where site investigations will be performed. This selection will be based on very preliminary evaluation of the feasibility of a deep repository in different regions in Sweden and in some specific municipalities. These evaluations are based on already existing geological data and involve studies of how a repository can be constructed and how it would influence the studied areas and municipalities, with regard to environment, society, infrastructure, transportation, tourism, etc. According to present plans the siting stage will continue until 2001, after which the two areas will be selected. One prerequisite for starting site investigations is that the investigation plans are acceptable to the local community.

2 Site investigation stage

2.1 General goals

The aim of the site investigation stage is to collect site-specific data at two sites and evaluate the sites with regard to the feasibility of constructing a deep repository for spent nuclear fuel. At least one of the two sites must fulfil the requirements of long-term safety, suitable preliminary layout, and acceptable impact on the environment and the community. SKB will select one of the two sites as the preferred repository site and prepare an application for permission to carry out detailed characterization to be submitted to the government. The application will be reviewed under both the Act Concerning the Management of Natural Resources and the Act on Nuclear Activities, which indicates the importance of the site investigation stage. Besides the technical results, of which the safety report is the most important, the EIA process, in which representatives from SKB and the community will participate, will be an important instrument for site selection and application review.

The aim of the subsequent detailed characterization is to verify the feasibility and safety of the deep repository on the selected site. Detailed characterization involves

construction of tunnels down to the repository level and extensive investigations and experiments from tunnels and boreholes. The design studies involve a more detailed repository layout, and a new safety assessment will be conducted before a permit for construction of deposition tunnels and start of repository operation is issued.

2.2 Activities during the site investigation stage

During the site investigation stage a huge amount of site specific information will be collected and evaluated. The areas of endeavour will be:

- geoscientific investigations and modelling,
- design and layout studies,
- performance and safety assessment,
- environmental and societal impact studies,
- geoscientific site evaluation.

The geoscientific investigations are the most extensive of these activities and will produce a large amount of data, which will be used for geoscientific modelling and further analysis and evaluations in the other activities. The intention is that all these activities will be conducted in parallel, enabling feedback obtained from the analysis activities to serve as guidance for the continued geoscientific investigations.

The role of organizing the information exchange will be allocated to the geoscientific site evaluation. During the ongoing investigations, the geoscientific site evaluation will act as an engine for the interactive site investigation process, see Figure 2. Geoscientific factors and criteria for site evaluation are discussed by Ström et al (1998).

3 The geoscientific investigation programme

3.1 Characterization guidelines

The goals of the geoscientific investigations for the deep repository are:

- The investigations should provide a geoscientific understanding of the site and its regional environs with respect to the present-day situation and natural ongoing processes.
- The investigations should provide the necessary geoscientific data for a site-adapted design of the deep repository and for assessment of the deep repository's long-term performance and radiological safety.

What data and information are then needed for a geoscientific understanding, for the performance and safety assessments and for the design and layout studies? Knowing this is of the utmost importance for preparation of the site investigation programme. SKB has therefore identified and structured the need of geoscientific information in a "parameter" report (Andersson et al, 1997). For each modelling subject area, all



Figure 2 Activities and interactions during site investigations.

parameters (geoscientific data, properties, conditions, etc.) which in one way or another will be used during the site investigations are presented and discussed according to their importance for:

- long term safety; with regard to the function of the engineered barriers (spent fuel, canister, buffer, bedrock) for the general safety functions (isolation, retardation and biosphere),
- repository design; with regard to layout, construction and working environment,
- geoscientific understanding of the site.

The report also discusses how the parameters will be used in the geoscientific model description of the site and presents the modelling structure for which the investigated sites will be characterized, see Figure 3:


Figure 3. Geoscientific models and how these models are utilized for safety and suitability assessment.

3.2 Development of the investigation programme

The required information is presented (and structured) in the parameter report. We have a toolbox of methods, instruments, experience and know-how available for measuring, analyzing, evaluating and modelling the potential host rock conditions. Other kinds of input which have to be taken into account are site-specific conditions, technical and administrative conditions and programme strategies. Aspects of importance for the programme are:

- Goal-oriented programme; The general objectives of the site investigations will be broken down into detailed goals for the different subject areas as well as for the investigation stages.
- Adaptation to site-specific conditions; The site investigation programme can be specified to a certain degree before sites are selected. However, site specific conditions, such as amount of exposed rock, already existing data, etc., must be known to devise the site-specific investigation programme.

Logical investigation stages will be based on the client's need, information will be transferred when decisions have to be taken (such as selection of central site area, decision on preliminary layout, etc.) and when feedback is desirable for new investigation steps.

- Characterization on different scales The characterization for the site investigation will be done on the regional scale and on the local site scale. The regional area will be in the order of 50 km² while the site area for the local scale model will be approximately 5 km².
- Investigation/modelling in subject areas Modelling subject areas were presented above. The execution of the investigations will be organized in the subject areas geology, hydrogeology and hydrochemistry, because these are the most work intensive subject areas. Rock mechanics and thermal modelling will fall under geology, while activities for transport modelling are related to hydrogeology and hydrochemistry. Notwithstanding this organizational structure, intimate interaction in planning, execution and modelling will ensure the development of integrated geoscientific models.
- Interaction within the geoscientific site evaluation Feedback from the "clients", i.e. the performance and safety assessments and design and layout, is of the utmost importance in ensuring that the right information is collected. The previously mentioned geoscientific site evaluation will be the tool for this information exchange.

3.3 Outline of the investigation programme

According to present plans the site investigation will be carried out in two main stages: initial and complete site investigation.

- The main purpose of the initial site investigation is to ascertain with relatively limited measures whether the judgements from the feasibility study are correct. The initial studies also aim at identifying where within a stipulated area the potential for a deep repository is greatest and thereby where the continued investigations should be concentrated.
- The main purpose of the complete site investigation is to characterize the site so thoroughly and completely that a fundamental geoscientific understanding is achieved and a site-adapted repository layout and assessment of long-term performance and safety can be submitted together with the application for a permit for detailed characterization.

The outline of the investigation programme, examples of typical investigations and requested results are shown in Figures 4 and 5 (SKB 1995, a).



Figure 4 Conceptual sketch of scope of an initial site investigation.

3.4 The role of geological discontinuities

As can be seen in the figures, the investigations are to a great extent aimed at the identification of discontinuities (fracture zones), due to the fact that repository layout will be guided by these geological elements, because of their importance for rock stability and nuclide transport. The importance of discontinuities for repository performance has resulted in a functional classification of discontinuities that SKB will use in the repository studies. The following classes are defined:

- Discontinuity of functional class D1 (Discontinuities influencing the siting of the repository) These discontinuities are not accepted within the repository volume.
- Discontinuity of functional class D2 (Discontinuities influencing the overall layout of the repository) These discontinuities can be accepted between main deposition areas in the repository.



Figure 5 Conceptual sketch of scope of a complete site investigation.

Discontinuity of functional class D3

 (Discontinuities influencing the layout of deposition tunnels and boreholes)
 These discontinuities can be accepted within deposition areas, but not in deposition holes.

 Discontinuity of functional class D4 (Discontinuities with no influence on the repository layout) These discontinuities can normally also be accepted in deposition holes.

In the geoscientific models the discontinuities are named according to their geometric size (length and width), as defined in the geological-structural model, see Table 1. The character of the discontinuities is described in the other models. One ambition of the site investigation is to identify and deterministically characterize all regional and local discontinuities, while local minor discontinuities and individual fractures will be characterized stochastically.

Table 1. Geoscientific classification and designation of discontinuities plus level of ambition for description in connection with site investigation (the dimensions are approximate).

Designation	Length	Width	Ambition for description
Regional discontinuities	>10 km	>100 m	Deterministic
Local discontinuities	1 – 10 km	5 – 100 m	Deterministic
Local minor discontinuities	10 m – 1 km	0.1 – 5 m	Stochastic (some determin.)
Individual fractures	<10 m	<0.1 m	Stochastic

There is no strict correlation between the geoscientific classes and the functional classes of the discontinuities, since functional importance (for mechanical stability, transport capacity, rock engineering aspects, etc.) is not solely dependent on geometric size. However, generally speaking, most of the regional, local, local minor discontinuities and individual fractures correspond to the functional classes 1, 2, 3 and 4, respectively.

4. Concluding remarks

The site investigation programme for generic sites is planned to be presented for review at the end of this year. With the intention of starting site investigations in 2001, the next few years will be used for detailed planning and preparation of the previously mentioned subject areas, characterization programmes, instruments, method instructions, and (when the candidate sites are to be selected) site-specific investigation programmes. Moreover, programmes for the geoscientific evaluation will be developed.

As is evident from this paper, the site investigation programme is based to a great extent on experience and results from the Äspö Hard Rock Laboratory. The extensive studies pertaining to verification of site investigation methods have been of particular importance.

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SITING FACTORS FOR THE SWEDISH DEEP REPOSITORY FOR SPENT FUEL

Anders Ström, SKB Karl-Erik Almén, KEA GEO-Konsult Johan Andersson, Golder Associates Lars O Ericsson, SKB Christer Svemar, SKB

Abstract

A project entitled *Siting factors and criteria for site evaluation* was initiated at the Swedish Nuclear Fuel and Waste Management Co. in 1997. The project comprises an important part of the work of siting and site selection that is being pursued within SKB. The purpose of the project is to create a logical structure for the continued siting work, and its results should also be able to be used to assist in evaluating sites. The project will thereby also provide a means – in accordance with the Government's decision regarding RD&D-Programme 95 – to obtain more detailed and quantified siting factors and criteria than those previously presented in the supplement to RD&D-Programme 92.

The overall goals of the project are to identify and quantify requirements and preferences regarding the properties of the rock and the soil from the perspectives of long-term safety, performance and planning and design of the rock works, and to identify siting factors and criteria. The latter should be able to be used to determine whether requirements and preferences are satisfied, both when screening sites for site investigation and after completed site investigation.

Presented requirements, preferences, factors and criteria must be acceptable to national and municipal authorities or others with influence over the siting work.

To start with, requirements and preferences regarding the performance of the rock in a deep repository have been clarified. These requirements and preferences are based on many years of experience of safety assessments and construction analyses within SKB. What is new here is the structuring that has been done, where a classification is made into different geoscientific disciplines, and the formalism that has been developed for the concepts *requirements, preferences* and *performance*. This is a prerequisite for a consistent and hopefully comprehensive set of requirements from a functional perspective.

Work has continued on siting factors (geoscientific evaluation factors) with reference to a coming site investigation programme. A geoscientific parameter that can be measured or estimated in site investigations is considered to be a suitable siting factor if either of the following conditions is met:

- · a direct requirements or a strong preference has been formulated for the parameter, or
- the parameter is expected to have a great influence on the results of one or more important performance analysis.

The project will be concluded during 1999.

Introduction

For the siting of a deep repository for spent nuclear fuel it is very essential for SKB to present clear siting factors and criteria for site evaluation. Detailed factors and criteria constitute an important basis for the evaluation of possible sites. At the same time siting factors have been required by the Government in connection with a decision on Dec 19, 1996, on account of SKB's RD&D Programme 95.

The following principal goals have been set for the project Siting Factors and Criteria for Site Evaluation:

- to identify and quantify requirements and preferences regarding conditions and properties of the rock from the perspectives long-term safety and technology.
- to identify geoscientific evaluation factors and propose criteria that can be used to determine whether requirements and preferences are satisfied and to compare sites prior to site investigation and prior to detailed characterization.

A prerequisite for the application of the criteria is the completion of survey and feasibility studies.

The starting point for the project are above all the comprehensive siting factors described in connection with the supplementation of the RD&D programme 92 /SKB, 1994/ and the work that has been done to identify the parameters which are important to determine when performing a geoscientific site investigation /Andersson et al, 1998/.

The function and safety of the deep repository must eventually be evaluated through an integrated safety analysis. The use of factors and criteria can never replace that. The result from the project can instead be used when making a geoscientific site evaluation. The main purposes of such an evaluation are as follows:

- to verify for the site in question that fundamental safety requirements and other essential technical prerequisites are met;
- that the deep repository is optimally adapted to the conditions and properties of the site.

The evaluation should also yield material permitting comparison of different sites, primarily with respect to long-term performance and safety, but also other geotechnical siting factors. The geoscientific evaluation of the sites should provide the background material needed for an application for a detailed investigation and the construction of a deep repository.

Requirements for the deep repository

To start with, requirements and preferences regarding the performance of the rock in a deep repository have been clarified. These requirements and preferences are based on SKB's experiences of safety assessments and construction analyses. What is new here is the structuring that has been done, where a classification is made into different geoscientific disciplines, and the formalism that has been developed for the concepts *requirements, preferences* and *performance*. This is a prerequisite for a consistent and hopefully comprehensive set of requirements from a performance perspective. Based on general requirements and preferences regarding safety and construction functions, these have been broken down into the disciplines geology, thermal properties, hydrogeology, rock mechanics, chemistry and transport properties. Detailing has been done for each discipline. Furthermore,

performance analyses have been identified by means of which it is possible to concretely define the performance requirements and which geoscientific parameters are relevant.

Figure 1 constitute an illustration of use of geoscientific modelling, the extent of the project and the relation to site evaluation.



Figure 1. The use of geoscientific modelling in performance and safety assessment is illustrated. The project identifies requirements regarding the rock properties of the deep repository at different levels.

Geoscientific evaluation factors

The concept *siting factor* is used in many connections when the siting of a deep repository is discussed. In the feasibility studies overall siting factors are used to decide whether an area is suitable for the siting of a deep repository. The factors are divided into the following main groups:

Safety	Siting factors of importance for the long-term safety of the deep repository
Technology	Siting factors of importance for the construction, performance and safe operation of the deep repository and for the transport system of the deep repository
Land and environment	Siting factors of importance for the use of the land and the general impact on the environment
Societal aspects	Siting factors linked to social conditions and social impact

In this study the concept *geoscientific evaluation factor* is used. This is a certain delimitation and specification indicating that there is a linking to a certain stage in the siting work and that technique and long-term safety are in focus. The evaluation factors constitute a subset of all the geoscientific parameters which will be determined in connection with a site investigation.

Requirements and preferences regarding the deep repository, and accordingly the rock, are defined above all with reference to the performance and not directly the separate parameter values. In the same way as for requirements and preferences regarding the performance of the rock, evaluation factors have been established for each geoscientific subject field.

A geoscientific parameter which can be measured or estimated during site investigations is considered to be a suitable evaluation factor if one of the following conditions is satisfied:

- a direct requirement or an essential preference has been defined for the parameter, or
- the parameter has an expected great influence on the result of one or more important performance analyses.

Based on a preliminary list of potential evaluation factors, there should also be a discussion of the level of knowledge which can or should be reached after the completion of a feasibility study, a site investigation and a detailed site characterization. It is not reasonable to choose a geoscientific parameter as evaluation factor, unless the parameter can be assessed.

Criteria for site evaluation

In the course of the continued work, criteria for site evaluaton will also be created. It should be possible to use these criteria to assess whether a site meets the established requirements and preferences or not. Regarding geoscientific parameters, criteria consist of characteristic values or fields of values for assessed evaluation factors. Regarding the performance of the deep repository, criteria consist of characteristic values or fields of values for the results of performance analyses. The criteria may change during the siting work, since information about sites may change. However, requirements and preferences will remain the same.

Criteria need to be linked to all available information at the current stage of the site investigation and to the decision-making situation in which they are to be used.

- Prior to a site investigation it is essential to be able to eliminate definitely unsuitable sites and also to be able to point out sites where there is a good prognosis that these sites will turn out to have suitable properties. At this stage criteria cannot be defined too clearly, in view of the limited information available about the properties of the rock at greater depths. The criteria should be used to select suitable sites for continued investigations. Checking if all requirements and preferences are met can only be made to a limited extent.
- After completing a site investigation it must be shown whether a site is suitable or not for a deep repository. At this point of time it may also be meaningful with criteria for comparing sites. Even if the result of the checking of the suitability of the sites is determined within the scope of overall analyses of safety and construction, the specified criteria should provide good guidance as to the outcome of such analyses.

Criteria for checking whether a site is suitable or not are based on the importance of the different evaluation factors and an assessment of the precision of current information. These criteria can therefore be founded on the evaluation factors that have already been established.

Even at this early stage it is possible to state that for certain evaluation factors it will be easy to define clear criteria. For other factors the criteria will have to be more complex. This applies for example to factors linked to the permeability of the rock. These factors influence different functions in different ways, they show significant spatial variability and an analysis of field data often implies extensive model work. The work to specify criteria will therefore not lead to specified value intervals for all

evaluation factors. On the other hand, it will be evident, for every factor, how information about them will be taken care of within the scope of perfomance analyses, in the results of the safety analysis or in the construction analysis.

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SITE SPECIFIC INFORMATION IN SITE SELECTION

Timo Äikäs and Aimo Hautojärvi POSIVA Oy, Helsinki, Finland

Abstract

The programme for the siting of a deep repository for final disposal of spent nuclear fuel was started already in 1983 and is carried out today by Posiva Oy which continues the work started by Teollisuuden Voima Oy (TVO). The programme aims at site selection by the end of the year 2000. The programme has progressed in successive interim stages with defined goals. After an early phase for site identification, five sites were selected in 1987 for preliminary site characterisation. Three of these were selected and judged to be best suited for the more detailed characterisation in 1992. An additional new site was included into the programme based on a separate feasibility study in the beginning of 1997.

Since the year 1983 several safety assessments together with technical plans of the facility have been completed. When approaching the site selection the needs for more detailed consideration of the site specific properties in the safety assessment have been increased. The Finnish regulator STUK has published a proposal for general safety requirements for the final disposal of spent nuclear fuel in Finland. This set of requirements has been projected to be used in conjunction of the decision making by the end 2000.

Based on the site evaluation all sites can provide a stable environment and there is evidence that the requirements for the longevity of the canister can be fulfilled at each site. In this manner the four candidate sites do not differ too much from each other. The main difference between the sites is in the salinity of the deep groundwater. The significance of differences in the salinity for the long-term safety cannot be defined yet. The differences may contribute to the discussion of the longevity of the bentonite buffer and also to the modelling of the groundwater flow and transport. The use of the geosphere as a transport barrier is basically culminated on the questions about sparse but fast flow routes and "how bad channeling can be". To answer these questions based on site specific information and evaluate the uncertainty is an important part of the discussion in the integrated work between site characterisation and safety assessment.

1 Introduction

The stepwise approach for site selection in Finland was included in the Council of State's Decision in Principle on the nuclear waste management in 1983. Based on this decision the site should be selected by the end of 2000 based on the systematic programme of identification, characterisation and evaluation. As the first step of this programme the bedrock of the whole country was evaluated during the years 1983-1985 to be able to locate potential candidate sites for the site characterisation in practice. Based on this work and the assessment of other factors, the second step of the programme, preliminary site characterisation was commissioned at five potential sites in 1987. This work was concluded at the end of 1992 in accordance with the overall programme. Since 1993 more detailed characterisation has been in progress on three sites, and a new additional site was included in the programme in the beginning of 1997.

At the three earlier sites, namely Kivetty in Äänekoski, Olkiluoto in Eurajoki and Romuvaara in Kuhmo, several deep boreholes have been drilled and comprehensive surface investigations already carried out since 1987. Therefore, very little additional information can no longer be achieved by surface based investigations at these sites. The fourth site, Hästholmen in Loviisa, is currently a target for an intensive investigation aiming at the evaluation of the site in parallel with the three other sites.

Which of the candidate sites will be selected for the final disposal is, of course, a sum of many factors. When deciding upon the site the following conditions have to be fulfilled

- the safety authority has to give the preliminary statement on the safety
- the local community has to accept the proposed project
- the Council of State has to approve the project and the Parliament has to ratify the decision

Before any nuclear facilities can be built in Finland the Council of State's Decision in Principle, based on the Nuclear Energy Act, is needed as the first step for implementation. This decision can be regarded as "a general permission" in the licensing process. At the later stages, the applications for construction license and the operation license are the following steps with their own processes.

The process for this decision making will be initiated by Posiva when submitting an application for this decision to the Government. Before the Government can make the decision it has to ask the approval of the communities which host the potential site candidates for the facility. The communities can exercise their right of veto on this matter in case they do not accept the facility. Before its own decision the Government has to also ask the Radiation and Nuclear Safety Authority (STUK) for the preliminary statement on the safety. When considering the decision the Government has to keep in mind the overall good of the society comprising the need for the facility, the suitability of the site and the environmental impacts assessed. In case the Government's decision is positive for final disposal the decision has to be subjected for the approval of the Parliament. This paper discusses the role of site specific information in the process of site selection. The site selection is, as presented above, a decision process involving also a dimension for political decision making. In this paper, however, the viewpoint is kept in the geoscientific information and in the evaluation of geosphere in the course of the site selection research programme.

2 Important Questions

The framework for the discussion in this paper has been sought by reiterating the following key questions for the site selection for final disposal, and these are

- what is the role of the geological barrier ?
- what are we looking for from a suitable geological environment?
- how good a geological barrier is needed?

When dealing with these questions the experience and information from the site selection research programme implemented in Finland is kept in mind. However, the questions above are not unique to the Finnish programme only but also discussed during the past years at the international arenas.

The purpose of the final disposal at the great depth in a geological formation is to remove the spent fuel from man's environment and place it out of reach of major disruptive processes. The geological formation is expected to provide an environment where the rates of natural processes affecting the canisters and spent fuel are slow and a thick layer of crystalline bedrock should as well provide an adequate shielding against a release of radioactive material from the waste itself.

The final disposal, however, is not based on the properties of the geological formation alone but consists of the multibarrier system planned for final disposal to isolate the waste from man's environment. The multibarrier system discussed in this paper comprises the fuel itself, the engineered barriers, that is copper canister and bentonite buffer, and crystalline bedrock as the natural barrier. The primary function of the bedrock is to provide stable mechanical and chemical conditions over the long periods of time so that the long-term performance of the engineered barriers is not jeopardised.

The main reason on the relative importance of the engineered barriers is that normally in the nuclear technology the safety can be based on the systems built from materials fully characterised and investigated, and if not so, the behaviour of which can be monitored to maintain the safe operation. At the great depth of the crystalline bedrock practically no technical improvements can be made regarding the long-term gross properties of the bedrock, and the basic question is how well it is possible to characterise the properties of the bedrock to be used in the preliminary repository design and in the site specific safety assessment. Due to the known heterogeneous nature of the geological environment and uncertainties associated the main emphasis for the safety assessments has been to develop reliance on the understanding of behaviour of the engineered barriers and the various processes in the near-field of the repository.

The contribution of the geological barrier of the deep repository to the safety is thus the physical protection of the disposal system as a whole. If something should happen the geological barrier should be able to restrict the possible radionuclide releases from the repository and through sorption and matrix diffusion be able to retard and retent the radionuclides escaped from the repository into the crystalline rock so that they do not form a risk in man's environment.

Finally, many safety cases have shown that the safety-related requirements are probably met by most sites identified and characterised in the crystalline basement areas (SKB-91, TVO-92, Kristallin-I, AECL, SKI-94, TILA-96) as candidate sites for a deep repository. This raises the question how good a geological barrier shall be as a whole. The waste will finally be placed in such bedrock volumes, characterised in great detail at depth, which most likely are able to provide an effective isolation, and bedrock sections which are regarded less promising are rejected from the repository volume.

In the following chapter it is described how the site information has evolved in the Finnish programme and how it has been used in the site evaluation so far.

3 Evolving Site Information

3.1 Identification of Potential Candidate Sites

The first step of the site selection research in Finland was to identify potential investigation sites to be able to select several sites for practical field investigations. In thinking the properties of a possible area for siting the following principles were applied (TVO 1992)

- a predictable environment was needed, preferably in all scales. This meant that homogeneity was preferred in rock types and more homogenous areas were judged to be more amenable to investigation
- low regional and local hydraulic gradients and low hydraulic conductivity of the bedrock were properties desired to ensure low groundwater flow rates and to provide longest possible transport times
- it was evident that the repository should be located away from potential tectonic zones and potential fast geosphere pathways
- the site to be selected should represent geological environment that has evolved only slowly and is currently relatively stable
- in order to minimise the possibility for inadvertent human intrusion the site should consist of common rock types, abundantly available

The geological starting point for the localisation of site candidates was to define "bedrock blocks" delineated by large fault zones interpreted from various sources of geological and geophysical information. The block areas were large, typically more than 100 km². Inside these block areas smaller blocks were analysed being simultaneously elevated areas representing groundwater recharge areas thus having as long as possible flow routes.

It was evident that at this stage the site information from a greater depth was incomplete and was based mainly on the interpretation of various existing geological, hydrogeological, geochemical and geophysical materials. During the course of the work, applying the principles mentioned above, it was obvious that the potential areas identified as an outcome of the studies became rather similar in their properties. This has to be kept in mind when discussing possibilities for later comparisons.

3.2 Preliminary Site Characterisation

Five areas were selected for the preliminary site characterisation in early 1987 (TVO 1992). These areas were selected from a great number of potential candidates. The sites represented different geological main units of the Finnish Precambrian bedrock in various parts of the country.

When considering the sites for selection the question of acceptance of the local communities was taken into consideration by having discussions with communities which had a candidate site within its territory. The purpose of these discussions was to identify the communities willing to cooperate at this stage and ensure that the communities allow the start of field investigations for preliminary characterisation. In judging the potential sites also possibilities for practical site exploration were considered.

In the course of the planning the programme for preliminary characterisation for the years 1987-1992 attention was drawn to following

- investigate the structure of the local bedrock to define the possibility for physical isolation of the engineered barrier system of the deep repository in the suitable bedrock volumes
- investigate the properties of the site to be able to model the potential groundwater fluxes through the repository and evaluate their significance
- investigate the groundwater chemistry to evaluate the impacts on the engineered barrier system
- study into long-term stability of tectonics, hydrogeochemistry and hydrogeology
- study into constructional and operational feasibility for the assumed amount of the waste

Based on the investigations at the sites it was possible to evaluate the gross properties of the bedrock. The geological features, geochemical conditions and hydraulical proper-

ties were good regarding the final disposal. The analysis exposed that each site candidate in principle could host a repository and no adverse properties existed. In the modelling of the bedrock structure some of the candidate sites were judged more complex than others (TVO 1992). The degree of certainty in interpreting results and inferring meaningful information from these for developing structural models was one of the important factors when judging the success for further site characterisation. The expectations to be successful in the further investigation was the reason for excluding two of the sites from the programme.

In the analysis of the groundwater flow a large contrast in flow distribution between averagely fractured rock volumes and fractured zones was assessed. The mean flow rates in the intact, averagely fractured, bedrock were estimated to be very low. The problem of faster pathways, however, was noted and in the safety assessment TVO-92 (Vieno et al. 1992) they provided a potential by-pass of the geological barrier as a conservative way to assess the safety of the deep repository. It was evident that the detection and analysis of fast pathways should become a significant part for the further site characterisation. The question "how bad can channeling be" was raised.

3.3 Detailed Site Characterisation

The current stage started in 1993 and aims at site selection in the year 2000. This eight year period has been divided into two stages for the years 1993-1996 and 1997-2000.

The work during the years 1993-1996 was divided into three sub-programs: 1) the baseline investigations describing the present conditions in the bedrock, 2) the additional characterisation for the acquisition of complementary data, and 3) the investigations for testing the earlier results and hypotheses to build confidence in existing understanding (Posiva 1996).

The baseline investigations have characterised the groundwater chemistry and its variations at the sites, as well as, summarised hydrological observations of Kivetty, Olkiluoto and Romuvaara. Saline groundwaters were found at Olkiluoto and results indicate that the salinity increases towards the depth. The state of the rock stress measured in deep boreholes correlates rather well with the general knowledge of rock stress in Finnish bedrock. Based on the interpretation of additional characterisation work carried out some complementary structural features were added, and some changes in earlier features were made to the bedrock models. The developments in the models did not, however, impede locating the vault at the desired depth in the bedrock.

The TILA-96 report (Vieno et al. 1996), a continuation and update of the TVO-92 safety analysis, confirmed that the planned system for spent fuel disposal fulfils the proposed safety criteria. Provided that no major disruptive event hits the repository, initially intact copper canisters preserve their integrity for millions of years and no significant amount of radioactive substances will ever escape from the repository. Impacts of potential canister failures have been analysed employing conservative assumptions, models and data. In the case of single canister failures, the results show that the margin to the proposed regulatory criteria is more than three orders of magnitude in the dose rate and more than four orders of magnitude in the release rates into the biosphere. Even

in the extreme cases, where all 1500 canisters are assumed to be initially defective or to "disappear" simultaneously at 10 000 years in the "worst possible location" in the repository, all the proposed safety criteria would be passed. When realistic modelling and data are used in the consequence analyses, the results show negligible releases and doses.

The TILA-96 report suggested for the further site characterisation and evaluation of the candidate sites that emphasis should be on three topics: I Evaluation of the geological structure and fracturing of the bedrock, II Identifying of bedrock volumes, where the repository could be constructed, and their assessment from the construction point of view, III Assessment of geochemical conditions (the role of brackish and sulphate-rich, saline, and very saline groundwaters).

In the present work which comprises also Hästholmen in Loviisa as a candidate site these questions have been introduced into two main areas, on the one hand there is the need to study the uncertainties related to geometry of fracture zones and fracture network of the site to be able to locate the potentially advantageous volumes for repository lay-out, and on the other hand improve the consistency between hydrogeology and hydrogeochemistry to understand the processes affecting the assumed stability of site candidates. This is needed because

- each site candidate has complex groundwater flow and solute transport paths
- has potential to fast pathways
- redox buffering capacity is difficult to demonstrate by direct investigations

The information from deep drillings and updating of the conceptual bedrock models enhanced the idea of the complexity of the geological barrier due to the heterogeneity. This leads to the fact that hydrogeological modelling will be associated with considerable amount of uncertainty and the transport in the geosphere will be dominated by properties of preferential flow paths such as WL/q ratio of each transport path. The question is how much site specific information can be produced to specify this parameter.

In the current work more emphasis has been put on hydrogeochemistry. The improved sampling techniques and increased number of samples have produced information on the existing chemical conditions at the sites. Overall, the sites seem to be in a postglacial quasi-static state containing "old" groundwaters, both fresh and saline, with efficient redox buffers. Hydrogeochemical modelling seems to be in accordance with structural geological information and hydrogeological interpretations. The work, however, is still underway. Paleohydrogeochemical techniques may provide some bounds for the estimation of future conditions to be used in the safety assessment.

The safety assessment work, aiming at TILA-99 report, has been integrated into the site characterisation together with some parts of the engineering aspects to enable a meaning-ful site evaluation.

4 Towards Decisions

4.1 Preliminary Safety Requirements

Finnish Centre for Radiation and Nuclear Safety (STUK) has prepared a proposal for general regulations concerning the disposal of spent nuclear fuel (STUK 1997). The proposal has been targeted to give support to the Council of State's Decision in Principle and site selection. After the period for commenting and preparation the general regulations are submitted to the Council of State for the approval.

Considering the siting of the deep repository the proposal contains among others following requirements:

- The geological characteristics of the disposal site shall, as a whole, be favourable for the containment for the nuclear waste to be disposed of. Areas having features that are substantially adverse to safety, shall be avoided in the selection of the disposal site.
- At the planned disposal depth, blocks of bedrock with suitable size and intactness shall exist for the construction of the repository. For the planning of the repository and to acquire data needed for the safety analysis, the host rock shall be adequately characterised by means of investigations performed at the planned disposal depth.
- The models and data introduced in a safety analysis shall be based on the best available experimental data and expert judgement. The models and data shall be selected on the basis of conditions that may exist at the disposal site in each time period considered in the analysis and they shall be adequately site specific and mutually consistent, taking account of the available investigation methods. The safety analysis shall, with good confidence, aim at overestimating the radiation impact likely to occur. The significance of uncertainties involved with safety analysis shall be estimated.

These requirements mean that the site selection can be based on the surface based investigations which are allowed to contain uncertainties. No extraordinary characteristics are required from a site to ensure the long-term safety of a deep repository for spent fuel.

4.2 Site Specific Information and Safety Assessment

Referring to the above mentioned requirements it is obvious that one important task for the upcoming safety assessment TILA-99 is to analyse the conditions necessary for safe disposal of each site. After this sites can be treated as candidates for further selection. In case the assessment would show signs of unacceptable conditions at a site, this site should be rejected from the selection process.

The requirements call for site specific information to be used in the models and calculations, however, on the other hand the safety analysis should be simultaneously conservative and aim at overestimating the possible impacts. This means that the direct comparison of the sites, using the results of safety analysis as such would not be very meaningful.

How good a geological barrier shall be, and what would make another site more advantageous than another? It is obvious that in the normal evolution scenario of the safety assessment the geological barrier at all sites can provide the basic demand of physical isolation from man's environment. The preliminary results of TILA-99 seem to support the earlier conclusions of TILA-96 (Vira et al. 1998) The most important characteristics of a suitable site are related to groundwater chemistry providing stable conditions for copper, and an environment for slow dissolution and low solubility of radionuclides. The other good properties of a site are if the probability for fast flowing features is low and the mineralogy of the bedrock is such that it can retent potential radioactive solutes in the groundwater. The technical concept, however, can be adapted to the geological conditions at depth so that it is possible to avoid, at least to a certain extent, fast flowing features.

The geological barrier is mostly needed if something unexpected would occur and weaken the good properties of the technical barriers. The question if some of the candidate sites would be more vulnerable for disruptive events in the future in the conditions of Finland causing major changes in the presently stable environment is not possible to predict quantitatively. In a case where a copper canister or several canisters would loose their integrity is decisive if this should happen next to a fast flowing feature. Based on the investigation methodology today it is not possible to say whether this would be more likely at some of the sites.

The most apparent difference between the candidate sites is that Olkiluoto and Hästholmen are presently located at the coast of the Baltic Sea, whereas Kivetty and Romuvaara are inland sites lying about 200 meters above the sea level. At the depth of 500 meters and downwards, groundwater is brackish or saline at Olkiluoto and Hästholmen, whereas it is fresh in Kivetty and Romuvaara. Salinity of the groundwater seems to affect to some degree negatively the near-field properties and retardation but on the other hand, salinity has been regarded often as a sign of very low or stagnant flow conditions and prevent humans of drinking such a water.

5 Summary

Site selection research has been a long process in Finland during which the site information has evolved gradually. During the process this information has been evaluated also by the means of safety analysis, starting from studying the feasibility of the final disposal based on generic information and ending up using the site specific properties aiming at assessing the bedrock volumes suitable for repository purposes.

The process has shown that the differences in the main properties of the bedrock in the different parts of Finland are rather small and similar suitable bedrock volumes can be identified at many sites. The citizens in the communities, as well as, the other decision

makers have their primary interest, however, in the safety of the final disposal and it is understandable that the idea of the "best possible site" is supported. Therefore the importance of small differences in site information have to be studied, evaluated and explained in the process.

The main role of the geological barrier is to provide an effective isolation of the waste, and we are looking forward mostly to mechanical and geochemical stability into the future from the geological environment at the site to be selected. Is any of the present sites more or less favourable than others comes down to a question of uncertainty. How well are we able to find and assess properties of suitable bedrock volumes at a particular site is one of the important questions ?

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The 3rd Aspö International Seminar

Posters

QUANTITATIVE DETERMINATION AND MONITORING OF WATER DISTRIBUTION IN ÄSPÖ GRANITE

Ulrich Zimmer

Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) mbH, Braunschweig, Germany

Abstract

To identify possible zones of two-phase-flow and the extension of the excavation disturbed zone, geoelectric measurements are conducted in the ZEDEX- and the DEMO-tunnel. The electric resistivity of a hard rock is usually determined by its water content, its water salinity and its porosity structure. By calibration measurements of the resistivity on rocks with well known water content, a relation between resistivity and water content for Äspö granite is determined. This relation is used to correlate the insitu resistivity with the water content of the rock. To determine the in-situ resistivity between the ZEDEX- and the DEMO-tunnel an electrode array of nearly 300 electrodes was installed along the tunnel walls and in one borehole. With a semiautomatic recording unit which is operated by a telephone connection from the GRS-office in Braunschweig/Germany, the resistivity is monitored between and around the tunnels. To correlate the resistivity with the water content, the measured apparent resistivity has to be converted into a resistivity model of the underground. Since many thin water bearing fractures complicate this inversion process, the accuracy and resolution of the different inversion programs are checked before their application to the data. It was found that an acceptable quantitative reconstruction of the resistivity requires the integration of geometric information about the fracture zones into the inversion process. For a rough estimation of the position of possible fracture zones, a simple inversion without any geometric boundary conditions can be used.

Since the maximum investigation area is limited along a single tunnel for profile measurements, tomographic measurements were also applied to estimate the resistivity distribution between the ZEDEX- and the DEMO-tunnel. These tomographic measurements have a lower resolution than the profile measurements due to the required large computer power, but result in reconstructions that give an estimate of the resistivity distribution in this area without disturbing the rock or the hydraulic field. Although the extension of single water bearing fractures cannot be proved due to the low resolution, more regional variations, especially with time, are monitored very well.

1 Introduction

For the identification of zones with possible two-phase-flow, the knowledge of the water content of a rock is important. From the water content, the saturation can be estimated if the porosity is determined, too. For this purpose non-destructive methods have the advantage of leaving the hydraulic field undisturbed. Consequently, geoelectric methods are highly suitable for such a problem. The quantitative determination and monitoring of moisture distribution in low-porosity rocks with geoelectric resistivity methods has successfully been applied at the GRS-Braunschweig (former GSF-Braunschweig) since 1989. During the last years, the recording technique, the data processing and the interpretation were consequently improved which allows now the application of this technique to the difficult case of fractured rock.

2 The methodology of resistivity interpretation in fractured rock

The methods of in-situ resistivity mappings are well known and have not changed very much during the last years. Popular configurations like the Wenner layout or the dipoledipole layout are still in use. But with the introduction of high performance computers it is possible to improve the interpretation of the measured resistivities.

From the measured current and voltage values an apparent resistivity is computed. In seismic methods the influence of the rock on the properties of the measured parameters, e.g. on velocity or attenuation, can be confined to a small tube connecting source and receiver, the seismic ray. In resistivity measurements a much larger area contributes to the computed resistivity value. For this reason, this value cannot be addressed to a single point although this is done for the visualisation of the data. For the interpretation a resistivity model of the underground is necessary. The computation of the true resistivity from the measured apparent resistivity is called inversion. Usually this inversion process was done by comparing the apparent resistivity with computed model curves which results in a 1-dimensional resistivity model.

During the last years, several programs for a 2-dimensional inversion of resistivities have become available. They differ in their concept of integrating geometric and topographic information. After the inversion, the resulting resistivity model of the underground can be interpreted in terms of petrophysical properties. In a common hard rock the water content presents the most important contribution to its resistivity. For each rock a specific relation between the water content and its electric resistivity exists. This relation is also influenced by the value and structure of its porosity. Once this relation is measured in the laboratory on samples with well known water contents, the inverted true resistivity distribution in the underground can be interpreted in terms of water content. For such a quantitative interpretation, the reliability and accuracy of the used inversion programs have to be estimated.

2.1 Resistivity Mapping Using Wenner Configurations

Geoelectric mapping with the Wenner configuration (Fig.: 1a) is a well known geophysical method. In hard rocks such as granite, electrodes are cemented to the rock with a constant spacing. To measure the apparent resistivity of the rock, a known voltage is applied between two of these electrodes (A/B) inducing a current through the rock. As a result of this current, a voltage can be measured between two other electrodes (M/N). The spacing of the electrodes A-M-N-B is the configuration parameter a. From the induced current (I_{AB}) and the measured voltage (U_{MN}), an apparent resistivity can be calculated using equation (1).

$$\rho_a = 2 \cdot \pi \cdot a \cdot \frac{U_{MN}}{I_{AB}} \tag{1}$$

To correlate the resistivities with the water content of the rock, the apparent resistivities have to be inverted to yield the true resistivities. Only these true resistivities can be interpreted in terms of water content of the rock (figure 1b).







Fig. 1b: The methodology of geoelectric mapping, the processing and the interpretation of the measured values

2.2 2D-Inversion of Pseudosections

As a result of the resistivity mapping using the Wenner configurations, a distribution of apparent resistivities (ρ_a) for different layout parameters (a) and different mid points of the configuration (x) is obtained (Fig. 2). The visualisation of the measured apparent resistivities is called pseudosection. The distribution of the apparent resistivity values must not be interpreted in terms of water content because its only a rough estimate of the underlying petrophysical situation. For a quantitative interpretation this pseudosection has to be inverted.





Fig.2a: Synthetic Resistivity Model

Fig. 2b: Apparent resistivities for a synthetic model with fractures

At the moment (1998), only a few commercial programs for a 2-dimensional inversion of resistivity pseudosections are available. For a 3D inversion no commercial software is available although some universities are working on this topic. The two applied programs differ in their ability to integrate geometric boundary conditions into the inversion process. But the basic principle is the same in both programs: from the measured apparent resistivities, a model of the resistivity distribution in the underground is estimated. For this model, the theoretical measurements are calculated and compared with the real measurements. The difference is used to improve the model. This iteration is continued until a satisfying adaptation is achieved.

2.2.1 Inversion Result With RES2DINV

The inversion program RES2DINV is not able to integrate geometric boundary conditions into the inversion process. On the other hand it does not need such information in advance for an inversion. The inversion result (Fig. 3) for the synthetic data set (Fig. 2b) shows clear anomalies of low resistivities at 12 m, 21 m and around 37 m which are the positions of the low resistivity bodies in the artificial model (Fig. 2a). But in contrast to figure 2, a the background of the model is not homogeneous. Many small anomalies of high resistivity occur near the surface. Additionally, it seems that the low resistivity anomalies are accompanied by a high resistivity anomaly nearby. This result shows that in an environment with elongated thin anomalies with a high resistivity contrast to the background the inversion result of the program RES2DINV should only be used as a qualitative estimate of the position of the anomalies.



Fig. 3: Inversion (RES2DINV) result of the synthetic apparent resistivities

2.2.2 Inversion Result With RSXIP2DI

In contrast to the program RES2DINV, it is possible to integrate geometric boundary information into the program RSXIP2DI. An advantage of this method is that the degrees of freedom are reduced which simplifies the calculations. To get a satisfying adaptation of the values and a correct resistivity distribution of the underground, it is necessary to start with a good initial model. Especially the number and general positions of the different bodies are critical parameters of the model. Although it is possible to allow the program a variation not only of the resistivities but also of the position and shape of the bodies no additional body can be inserted during the inversion process.

In this example the smallest of the bodies, was (intentional) not integrated in the initial model. Consequently, the inversion result only tries to model two of the bodies. In the initial model all of the anomalies were perpendicular to the surface. The dip of the rightmost anomaly was only corrected up to a depth of approximately 4 m. This is an indication of the maximum depth of relevance of the model. With greater depths the resolution decreases and a very small anomaly like a water bearing fracture has only a minor impact on the measured resistivity values at the surface.



Fig. 4: Inversion (RSXIP2DI) result of the synthetic apparent resistivities

2.3 2D Inversion of Resistivity Tomograms

Since the profile measurements have only a small depth of investigation, tomographic measurements are used to estimate the more regional resistivity distribution between the ZEDEX- and the DEMO-tunnel. The principle of the resistance tomography differs slightly from the profile measurements. Between two electrodes a known voltage is applied. This voltage induces a potential field in the rock. This field is measured at other electrodes of the array. From many measurements with different positions of the input voltage, the resistivity distribution in the area surrounded by the electrodes can be computed. Since many such electrode configurations are possible in an array with nearly 300 single electrodes, model computations have been used to select the most expressive configurations. Computer power is the other limiting factor. With the actual software it is only possible to compute tomograms from arrays with 49 electrodes. For large areas, this lowers the resolution of the model. The electrode configurations used with the Äspö array are described in more detail in section 3.4.

2.4 Guidelines for Resistivity Interpretation in Fractured Rock

From the investigations on the resolution and accuracy of the different programs which are available some general guidelines for the application and interpretation of the resistivity method *in rock containing water bearing fractures* can be derived:

- 1. An inversion with the program RES2DINV should only be used as an estimate of the major resistivity structure.
- 2. Thin elongated anomalies with a high resistivity contrast produce a high **and** a low resistivity anomaly in the inversion result.
- 3. The resolution of profile measurements / inversions decreases with depth.
- 4. As much additional information as possible has to be integrated into the inversion process, e.g., number, position and shape of expected anomalies.
- 5. For a quantitative interpretation the fracture zones have to be modelled explicitly.

3 Quantitative Determination of Water Distribution in Äspö Granite

For a quantitative determination of the water distribution in the rock between the ZEDEX- and the DEMO-tunnel, an electrode array was installed. With this array and the described interpretation software, the resistivity distribution around and between the tunnels was determined. To correlate the electric resistivity with the water content of the rock, laboratory measurements were necessary. With the installed array, the automatic recording unit, the remote control from the GRS-office at Braunschweig / Germany, and the laboratory measurements a quantitative determination and monitoring of the water distribution in this area were possible.

3.1 Resistivity - Water Content Relation for Äspö Granite

For the quantitative determination of the water content in Äspö granite, the knowledge of the relation between resistivity and water content for this specific rock is necessary. This relation was measured in the laboratory on samples with known water content. The results are shown in figure 5.



Fig. 5: Relation between water content and resistivity measured on Äspö granite samples with well known water content

3.2 Multi-Electrode Array at Äspö

For the determination of the resistivity and the water content between the ZEDEX- and DEMO-tunnel, 263 electrodes on 4 profiles were installed on the walls of the tunnels around this area; 111 electrodes in the ZEDEX drift, 42 and 10 electrodes in the access tunnel, and 100 electrodes in the DEMO-tunnel (Fig. 3). The electrodes on these profiles are 5-cm-long steel pins. They were cemented in small 3-cm-deep boreholes. The spacing between the electrodes was 0.5 m. To cover the fourth side of the area, another 36 electrodes were installed in a 40-m-long borehole. Since the borehole diameter is sufficient only for a limited number of cables, the distance between the electrodes is 1 m. All these electrodes are connected with a single cable to the automatic recording unit in a container at the end of the DEMO-tunnel which is controlled via a telephone line from the GRS-office in Braunschweig. The data were transferred via this telephone connection, too. This allows a high frequency of measurements. Although one reading lasts only 15 seconds, up to 8 hours are necessary to get a complete mapping of the ZEDEX or DEMO-tunnel. After some experiments it was found that the input voltage could be reduced to 50 V for all measurements.



Fig. 6: Distribution of the electrodes around the ZEDEX- and the DEMO-tunnel

3.3 Results of Geoelectrical Mapping

The results of the geoelectric mappings presented here are only an example for a single data set from each tunnel. The results have been obtained by an interactive modelling of the fractures. These fractures can be observed on the walls of the tunnels.

3.3.1 Demonstration-Tunnel (K)

The results from the DEMO-tunnel show six different fracture zones (Fig. 7). The topography included in the model is only approximated but the exact measurements from the Äspö-survey department are now available and will be integrated in further interpretation. However, it is already shown that the maximum topography in the Äspö tunnels is not expected to have a significant influence on the inversion results.

The resistivity of the background rock in the model is about 1000 Ω m. According to the laboratory results, this correlates to a full saturation of the intact rock. In contrast to this background, the fracture zones are modelled with a much lower resistivity of less than 100 Ω m. A more precise reconstruction is difficult because of the extremely high resistivity contrast which is limited only to a very small area. A slight variation in one of these parameters has, at least near the surface, a great impact on the other parameters.

One of the modelled fracture zones (the fourth from the left) has a slightly higher resistivity than the others. This is an indication for less water and a lower extension of this zone. Since it is difficult to estimate the absolute error of the model in this situation a quantitative interpretation of the resistivity in the fracture zone in terms of water content does not seem possible at the moment.

Besides the resistivity in the fracture zones, it is remarkable that no additional layer near the surface is necessary to explain the measured data in this model. This is an indication for only a small or even not existing excavation disturbed zone. At least, the excavation disturbed zone is not as big as it was suggested by the inversion results from the RES2DINV program. This program has difficulties with the exact inversion of thin elongated anomalies which are perpendicular to the profile.





3.3.2 ZEDEX-Tunnel (Z)

The inversion results from the DEMO-tunnel are very similar to the results from the ZEDEX-tunnel. The resistivity of the background is around 1000 Ω m and the water bearing fracture zones which are obvious at the surface are modelled explicitly. In contrast to the DEMO-tunnel, however, it is necessary to model a body near the surface with slightly higher resistivity. The reason for this anomaly cannot be a hidden water bearing fracture zone since the anomaly is very shallow. This anomaly is an indication for an excavation disturbed zone.



Fig. 8: Inversion result of the DEMO-tunnel profile measurements (06. Jan. 1998)

3.4 Resistivity Tomograms

For this method, the measuring configuration differs slightly from Wenner-mappings. The input electrodes (A, B) and the output electrodes (M, N) are arranged as single dipoles (Fig. 11). For a complete data set, the position of the input dipole (A, B) is fixed and the output dipole (M, N) is moved around the area to be investigated. Afterwards, the input dipole is moved to another position, and the measurements are repeated.



Fig. 9: Principle of dipole-dipole measurements and example of tomographic reconstruction.

Since a complete data set of all possible configurations from a multi-electrode array with 299 electrodes would exceed the capacity of the used inversion program, the number of configurations has to be reduced. In this case, model calculations have shown that a data set with 300 selected values should give a good estimate of the water content in the rock.

Since the capacity of the inversion software is limited to 49 electrodes, the resolution of the model is rather low with only 2 m x 2 m (Fig. 10). This is too low for an explicit modelling of the water bearing fractures in this area with an extension of only a few centimetres. But due to the large resistivity contrast they have an influence on the overall reconstruction of the resistivity distribution. Since the accuracy of the model is highest near the electrodes, the low resistivity anomalies in this part give an indication of the positions of the fracture zones. However, a proof for the connection of water bearing structures in this area is not possible with this resolution. Although the fractures can not be modelled explicitly, their changes in water content can be estimated by changes in the tomographic reconstruction with time.

4 Summary and Conclusion

Developments of the geoelectric instruments and the inversion software of resistivity measurements have improved the quantitative interpretation of the in-situ resistivity and related petrophysical parameters such as water content. Although a rock with water bearing fracture zones is still the limit for a justified quantitative interpretation, it is possible to get estimations of the water distribution in the rock with this method without disturbing the hydraulic field.

To obtain an optimum inversion of the measured data, an explicit modelling of water bearing fractures is necessary. For the special case of the Äspö geoelectric array, the topography along the tunnel walls is neglectable. Interpretations with the program RES2DINV imply additional positive anomalies besides water bearing fractures which lead to a wrong interpretation in terms of water content. With the program RSXIP2DI, these effects are eliminated by integrating the geometric boundary conditions. Indications for an excavation disturbed zone are found but, if existent, it is much smaller than predicted from RES2DINV inversions.

HRL ÄSPÖ - TWO-PHASE FLOW EXPERIMENT - GAS AND WATER FLOW IN FRACTURED CRYSTALLINE ROCK

Abstract

Gas generated from radioactive waste may influence the hydraulic and mechanical properties of the man-made barriers and the immediate surroundings of the repository. Prediction of alteration in fractured crystalline rock is difficult. There is a lack of experimental data, and calibrated models are not yet available. Because of the general importance of this matter the Federal Ministry for Education, Science, Research and Technology (BMBF) decided to conduct a two-phase flow study at HRL. ÄSPÖ within the scope of the co-operation agreement with SKB.

Within the presentation an overview of field experiments and modelling studies scheduled until end of '99 are given. Conceptual models for oneand two-phase flow, methodologies and with respect to numerical calculations necessary parameter set-ups are discussed.

Common objective of in-situ experiments is to calibrate flow models to improve the reliability of predictions for gas migration through fractured rock mass. Hence, in a defined dipole flow field in niche 2/715 at HRL Äspö effective hydraulic parameters are evaluated. Numerical modelling of nonisothermal, two-phase, two-component processes is feasible only for twodimensional representation of a porous medium. To overcome this restriction, a computer program will be developed to model threedimensional, fractured, porous media.

Rational aspects of two-phase flow studies are for the designing of geotechnical barriers and for the long-term safety analysis of potential radionuclide transport in a future repository required for the licensing process.

H. Kull, GRS, L. Liedtke BGR, Germany

GLOBAL THERMO-MECHANICAL EFFECTS FROM A KBS-3 TYPE REPOSITORY

Eva Hakami and Stig-Olof Olofsson Itasca Geomekanik AB, Stockholm, Sweden

Abstract

The objective of this study has been to identify the global thermo-mechanical effects in the bedrock hosting a nuclear waste repository. Numerical thermo-mechanical modeling using distinct element models (*3DEC*) was performed. The number of fracture zones, the heat intensity of the waste, the material properties of the rock mass and the boundary conditions of the models were varied. Different models for multi-level repositories were also analyzed and compared to the main single-level case. Further, the global influence from the excavation of repository tunnels and deposition holes was examined by introducing weaker rock mass material properties in the repository region of one model.

The maximum compression stress obtained for the main model is 44 MPa and occurs at the repository level after about 100 years of deposition. Due to thermal expansion, the rock mass displaces upward, and the maximum heave at the ground surface after 1000 years is calculated to be 16 cm. In the area close to the ground surface the horizontal stresses reduce, causing the rock to yield in tension down to a depth of about 80 meters. The fracture zones show opening displacements at shallow depths and closing and shearing at the repository level. The maximum displacements are 0.3-2.5 cm for closing, 0.0-0.8 cm for opening and 0.2-2.2 cm for shearing.

The resultant stresses and displacements depend in large part on the assumptions made concerning the heat intensity of the waste. In the main model, an initial heat intensity of 10 W/m² is assumed, which gives larger effects than the case with 6 W/m². Another important input parameter for the analysis is the Young's modulus of the rock mass. In the main model, a value of 30 GPa is assumed. Higher values of Young's modulus give larger thermo-mechanical effects.

All multi-level repository layouts (with the same heat intensity on each level) give rise to higher temperatures than the single-level layout, causing the compressive stresses to increase more at the repository level. The multi-level layouts also cause a destressed zone extending in depth well beyond that induced by a single-level layout.

The *3DEC* model with altered properties at the repository region shows very similar results to the main model. The global effect from the excavated repository tunnels and deposition holes is therefore not significant. However, further numerical computations with repository tunnels and deposition holes modeled explicitly are needed to study the local thermo-mechanical response in the repository region.

1 Introduction

The Swedish nuclear fuel waste-disposal program plans to build a repository in deep bedrock. The proposed concept for the design of such repository is called KBS-3. In the safety assessment for the future repository, one of the tasks is to examine the expected conditions in the rock mass surrounding the repository. This is important because the rock mass functions as the outer barrier between the radioactive waste and the biosphere.

After the time of deposition, large amounts of heat will still be generated from the waste canisters. With time, the heat will spread out from the repository and cause the surrounding rock to expand. This also implies that the rock stress will redistribute both locally around the repository and at a larger distance on a "global" scale. This article will address the global thermo-mechanical effects from a KBS3-type repository and summarizes the work in this project. For more details see the summary report [Hakami et al., 1998].

The global thermo-mechanical effects from storing heat-generating spent nuclear fuel in the bedrock are difficult to predict precisely. The rock volume involved is very large and, even with extensive investigations, the detailed properties of the rock and the discontinuities would remain largely unknown. In addition, there is no previous experience from such heat-generating waste disposal. Therefore, the objectives of this study have been to use the existing knowledge of rock material and existing mathematical tools to try to identify, and possibly quantify, the thermo-mechanical effects that can be expected. While the study is not site-specific, an example of a realistic rock mass, the geology of Äspö, was used as a base for the model set-up.

In the first models, the rock mass was assumed to behave as a linear elastic continuum with isotropic and homogenous properties. In subsequent modeling, the numerical code *3DEC [Itasca, 1994]* was used. Using this code, further realism was introduced to the analysis by simulating the mechanical influence of major fracture zones in the repository area. *3DEC* models the response of a discontinuous medium (such as a fractured rock mass) as an assemblage of discrete blocks. The discontinuities are treated as interfaces between blocks, and each block is divided into a mesh of finite-difference elements. The behavior of the elements follows predefined constitutive laws.

Because the modeling requires simplifications concerning rock mass behavior, there is an uncertainty in the selection of appropriate material models and associated parameters. Where accurate parameters have been difficult to determine, a conservative approach has been taken — i.e., the parameters were selected such that the thermo-mechanical effects would not be underestimated. No effects from the groundwater are taken into account.

In the following, one of the *3DEC* models is referred to as the "main" model, as this is the model which is judged to be the most realistic in terms of rock mass properties.

2 Model Geometry

The 3DEC models were built within a block of 4000 x 4000 x 2000 m in size (see Figure 2-1a). This block has a fine element discretization close to the repository and a coarse mesh in the outer regions. For the model with a single repository level (main model), the area at the repository has an even finer discretization. The sides of the block are oriented parallel to the principal in-situ stress directions.



Figure 2-1 a) 3DEC model geometry and discretization regions. (Blocks in the foreground are hidden to reveal the inner parts of the model.) b) Model orientation and fracture zone geometry.

Figure 2-1b shows the location and orientation of the fracture zones considered in the 3DEC model. It can be noted that most zones are steeply dipping and oriented northeast-southwest. The most dominating fracture zones were selected from the SKB Äspö fracture network to be included in the model.

The repository was simulated as a grid of point heat sources. The location of heat sources was different in the model for the single-level repository (main model) and the multi-level cases. In total, seven different repository layouts have been compared. The thermal load area and the initial areal heat intensity was kept the same in each repository level for all layouts.

3 Thermal and Mechanical Model Properties

3.1 Thermal model

The heat-release function applied is defined by the following equation [Thunvik and Braester, 1991].:

$$\frac{Q(t)}{Q_0} = \left(\alpha_1 e^{-\alpha_2 t} + (1 - \alpha_1) e^{-\alpha_3 t}\right)$$
(3-1)

where Q(t) denotes the time-dependent heat intensity,
- Q_0 denotes the heat intensity at the time of the deposition,
- t is the time,
- α_1 , $\alpha_2\,$ and α_3 are constants

The initial heat intensity of one canister at the time of waste deposition (Q_0) is assumed to be 2400 W. With the canister spacing used (40 m x 6 m), the corresponding initial areal intensity becomes 10.0 W/m².

The ground surface was modeled as a fixed temperature boundary. The initial temperatures in the bedrock were assumed to increase linearly with depth, from 7 °C at the ground surface to about 15 °C at 500 m depth.

The thermal properties are assumed to be isotropic and constant throughout the rock block. Thus, the fracture zones do not influence the thermal field. Influences from excavations, filling materials, heat convection by fluid flow or fluid buoyancy were not considered. The specific heat and expansion coefficient have been kept the same in all models. The thermal conductivity was 3.0 W/m °C in the main model.

3.2 Mechanical model

The in-situ stress state, as measured at Äspö, is taken to be the initial stress conditions. The major principal stress is nearly horizontal, with a bearing of N40W; the intermediate stress is subhorizontal, and the minor stress is close to vertical. Based on the measured results, the initial stresses were assumed to vary linearly with depth. The upper surface (ground surface) was modeled as a free surface; all other boundary surfaces were restricted to zero normal displacement.

A Mohr-Coulomb plasticity model was used for the intact rock blocks, and an elasticplastic constitutive model with Coulomb slip failure was used for the fracture zones. The input mechanical property parameters used for the rock blocks in the main model are given in Table 3-1. The alternative values used are given in parenthesis.

Parameter	Value	
Young's modulus [GPa]	30 (60)	
Poisson's ratio	0.22	
Cohesion [MPa]	5	
Friction angle [°]	30	
Tensile strength [MPa]	0 (8.7)	

Table 3-1Rock mass properties used in the models.

The cohesion is assumed to be zero and the friction angle for the fracture zones equal to 20°. Each fracture zone stiffness was assumed based on the esstimated zone width (for further detials, see [Hakami et al. 1998]) and the parameters have been kept the same in all analyses. The knowledge about the mechanical properties of fracture zones is poor, however, because it is difficult to get field information on structures of this size. It can be noted that the fracture zones are here simulated as single continuous features, transecting the entire model.

4 Results

It was found that, at the repository level, the peak temperature was reached at about 200-400 years after deposition. Figure 4-1 shows the temperature distribution along the same vertical line for different layouts of the repository. It can be noted that, as expected, the multilevel repositories cause the highest temperatures at the center of the repository. Smaller separation between the levels also gives higher maximum temperatures, due to the influence between the levels. The layout 3_50 (three levels with 50-meter separation) thus causes the highest temperatures among the layouts studied.



Figure 4-1. Temperature distribution along the vertical scanline through the center for the different layouts, after 400 years of deposition. (1_SQ denotes the "main model", with a square single-level repository at 500 m depth; 2_100 denotes a two-level repository with 100-m separation between levels, etc; 2_REC denotes a model with two rectangular levels with 100 m separation)

The calculated stresses for each time analyzed were collected at element zone centroids closest to the specified points along a vertical scanline. Figures 4-2 shows how the major principal stress changes with time along this vertical line.

After 50 years of deposition, an increase in major principal stress of about 12 MPa is calculated, at the level of the repository. Between the times 400 and 1000 years after deposition the major stress, in this area, starts to decrease slowly and at 1000 years the major stress lies about 10 MPa higher than the initial stress. In areas far from the repository, the stress changes are largest at the latest time analyzed (1000 years). Also, the



change in minor principal stress continues to increase within the time span analyzed. At 1000 years, the minor stress has increased about 4 MPa at the repository level.

Figure 4-2. Major principal stress along the vertical scanline for the main model, 1_SQ.

In the rock mass close to the ground surface, the principal stresses decrease compared to the initial state of stress. At 1000 years, the major principal stress has decreased to about zero from the initial value of 5 MPa. During the thermo-mechanical process, there is also a reorientation of principal stresses such that the minor principal stress becomes horizontal close to the ground surface, while it is vertical at greater depth.

The thermal expansion of the rock mass surrounding the repository gives rise to a corresponding rock mass displacement in the outward direction. The heave of the ground surface increases with time as a larger volume of rock mass expands. The magnitude of the heave also depends on the geometry of the repository. The two cases giving the highest values have their upper levels closest to the ground surface, as compared to the other layouts. The smallest heave (16.5 cm) was obtained for the single-level repository.

As already mentioned, the thermal expansion and the corresponding rock displacements cause a destressing of the rock mass at shallow depth. In the main model, where the rock mass is assumed to have no tensile strength, the stress decrease leads to tensile yield in this area. Other models show a similar pattern, but with tensile yield down to different depths.

The fracture zone displacement varies both spatially, over the fracture zone area, and with time. Figures 4-3 show an examples of calculated fracture zone normal displacements plotted in a vertical section of the model. The largest closing displacements can be seen at the repository level; displacements in the opening direction occur at shallower depth. Differences in location, orientation and stiffness explain the differences in displacement magnitudes between fracture zones. The largest displacements calculated on each fracture

zone are compiled in Table 4-1. (These maximum values may refer to different times analyzed and different repository layouts, but are all from models with an initial thermal load of 10 W/m² and E = 30 GPa.)



Figure 4-3 Normal displacements of fracture zones. Note that vector lengths correspond to the magnitudes (i.e. closing at depth and opening close to ground surface).

It can be noted from Table 4-1 that all maximum displacements are in the range from zero to five centimeters, where the closing displacements are the largest and the opening displacements smaller. These displacement magnitudes should be related to the width of the deforming fracture zones, which are up to 30 meters. The pattern of fracture zone displacement is fairly consistent between different models analyzed, which should be expected since the stiffness of the fracture zones was not changed.

Table 4-1	1 Maximum observed displacements of the fracture zones.		
Fracture	Maximum Closure	Maximum Opening	Maximum Shearing
Zone	[cm]	[cm]	[cm]
EW-1n	2.7	0.8	1.4
EW-1s	3.2	1.0	1.4
EW-3	2.2	0.8	1.1
EW-7	0.2	0.0	0.2
NE-1	4.5	0.9	2.7
NE-2	1.8	0.5	1.0
NE-3	2.2	0.3	1.4
NE-4	0.4	0.2	0.5
NNW-4w	2.5	0.5	1.0

5 Sensitivity Analysis

5.1 Geological model set-up

Modeling with increasing number of fracture zone geometries were performed to investigate the influence of the fracture zones. A continuum model produces the largest stress increase at the repository level. The stress increase gradually becomes smaller with more fracture zones included. Even though the number of fracture zones in the model influences the stress magnitudes, no major stress rotations or redistributions can be seen as a result of fracture zones cutting through the rock mass. The explanation to this is that most fracture zones behave elastically within the time span studied and that all model boundary surfaces (except for ground surface) are fixed in their normal directions.

5.2 Boundary conditions

Ideally, the size of a numerical model is large enough so that the boundary conditions will not affect the area of interest. However, in this study it was expected that a change in boundary condition from fixed normal displacement to fixed normal stress conditions would give slightly different results. Therefore, these two different cases were compared. The results show that stress levels change slightly with changed boundary condition. In general, the fixed displacement condition gives higher stress levels. Stress boundaries give a slightly deeper area of tensile stresses. The stress boundary case also results in 20-40 % larger opening and shear displacements at the ground surface for some of the fracture zones. At the repository horizon, there is a slight decrease in displacements for some of the fracture zones for this case.

5.3 Material properties

In some of the *3DEC* models, the rock mass was assumed to have a tensile strength of 8.7 MPa. It was judged, however, that a material without tensile strength would better represent the actual rock mass material, since the blocks in the *3DEC* models are not simulating intact rock blocks but, rather, rock mass volumes between fracture zones. Analyses performed with and without tensile strength were thus compared; the main difference was, as expected, seen in the stresses in the rock mass close to the ground surface. Without tensile strength the stress may not go below zero.

A similar comparison was also carried out for a change in the Young's modulus of the rock mass blocks. One of the two values used was 60 GPa, which is regarded as a high value; the other value chosen was 30 GPa. The differences in results between these two cases are quite large. The maximum major principal stress at the repository level is, for example, 44 MPa using the lower value and about 52 MPa with the high value. The depth to which tensile stresses occur, for the case with E = 30 GPa, is reduced by about 50%. (A tensile strength of 8.7 MPa was assumed.) Accordingly, a major reduction of the fracture zone displacements are obtained with the lower modulus.

5.4 Effects of excavation openings

In the main modeling work for this study, the repository was only simulated in terms of the thermal load from the heat generating canisters. To investigate how much the excavation openings could influence the thermo-mechanical effects, on a global scale, an additional *3DEC* analysis was performed. In this model a tabular region of 24 height was given lower material properties to simulate the more compliant behavior of the repository horizon due to the excavations. A two-dimensional distinct element model was used to calculate the most appropriate "equivalent" material properties to be used. The Young's modulus was reduced from 30 to 28 GPa and the friction angle from 30 to 19 degrees.

The stress distribution and displacements calculated are almost identical to the main model in areas outside the repository region. But in the elements of the repository region itself yield occur in this case with lower material strength. A very small influence on the global behavior can be seen in ground surface heave. After 1000 years, the case that considers excavation openings has an insignificantly higher value than the main model.

6 Discussion

The thermal conductivity of the rock mass restrains the heat front from moving quickly. Therefore, the heave of the ground surface continues to grow slightly even after 1000 years. Calculations in this study have, however, not been extended beyond 1000 years. To fully monitor stresses and displacements covering the peak response and the cooling phase, a somewhat longer time period should be studied.

The assumptions about the constitutive model and the input parameters influence the modeled rock mass behavior, particularly at the ground surface. The most important parameter in this respect is the Young's modulus. A value of 60 GPa for Young's modulus is in the order of the intact rock modulus. However, rock mass blocks with sizes of hundreds of meters would have lower stiffness than intact rock, due to the fractures. It is therefore likely that the lower value (30 GPa) used in much of this study is more appropriate for prediction, although this is not the most conservative choice.

Based on the observations of the Äspö geology, it may also be noted that the "geological models" considered in this study all have fracture zones with subvertical dip. In a more general study, one could consider also having horizontal or gently dipping structures located between the repository and the ground surface and/or having a rock mass with depth-dependent Young's modulus.

During the long-term thermo-mechanical loading of the rock mass in its global scale, the fracture zones undergo closure, opening and shearing displacements. From the perspective of the mechanical stability of a repository, these movements are advantageous, since some of the stresses are relieved. Closure of the fracture zones in the neighborhood of a repository is also advantageous with respect to hydraulic properties. On the other hand, the opening of fracture zones at shallow depth may enhance the groundwater movement in this area. Shear displacements of the fracture zones may or may not play a significant role on the groundwater movement.

As a part of the safety assessment, criteria concerning acceptable levels of displacement must be determined for the fracture zones. Because the actual effects on the transport properties from fracture displacement are difficult to determine, one possible criterion could be that limited fracture zone displacements in the opening direction are accepted if they occur in areas where the properties of the rock mass are not critical for the assessment.

Because there is great general uncertainty in selecting input parameters for a large rock area, the span of potential thermo-mechanical effects becomes large. The selection of properties of the repository region should also be viewed in this context. The reductions estimated, due to excavation openings, may well be of the same order as the natural variation of strength parameters in the rock mass.

In the present "global scale" study, the approach was that the effect of excavation openings could be simulated in the model with a tabular region of continuum material. Also, the heat flux in this global study was simplified geometrically to point heat sources. Furthermore, the temperatures and stresses reported here refer to a scanline in the model about 20 meters away from the canisters. It should therefore be noted that detailed distribution of temperatures, and thermo-mechanical effects near the repository, must be discussed based on modeling on a smaller scale.

7 Conclusions

For a single-level repository, the temperature reaches a maximum of 70 °C during 100–400 years after deposition, considering a vertical scanline between the tunnels. Far from the repository, the temperature still increases slightly after 1000 years of deposition. The principal stresses increase near the repository, closing the fracture zones at that vicinity. The maximum principal stress obtained for the main model is 44 MPa and occurs at the repository level after about 100 years (The main model has E = 30 GPa). The reduction of the minor principal stress at the ground surface causes the rock to yield in tension down to a depth of 80 meters. The fracture zones also exhibit opening displacements at shallow depths due to the normal stress decrease. Closer to the repository, the fracture-zone displacements are closing and shearing. The magnitudes of maximum displacements for the different fracture zones, are 0.3-2.5 cm for closing, 0.0-0.8 cm for opening and 0.2-2.2 cm for shearing, respectively.

The magnitudes of the stress changes and displacements calculated depend on the assumptions made concerning heat intensity and heat intensity function. For example, the major stress increases up to 50 MPa for 10 W/m² initial heat effect and up to 42 MPa for 6 W/m² (E= 60 GPa). Another important input parameter for the resulting thermomechanical effects is the Young's modulus for the rock blocks. For example, the closure of fracture zones around the repository decreases by 40% when the Young's modulus is lowered to 30 GPa from 60 GPa. Also, the stress release at the ground surface is less with the lower Young's modulus.

The predicted stress at the repository level becomes highest for a continuum, elastic assumption and gradually decreases as more fracture zones are included in the analysis.

The presence of major fracture zones in the rock mass could thus be important for the stress level reached at the repository, since peak stresses are reduced. Because it is difficult to determine the stiffness of a fracture zone, the magnitudes of predicted displacements are uncertain.

All multi-level repository layouts analyzed give rise to higher temperatures in the surrounding rock mass than does the single-level layout. This also causes the compressive stresses to increase more at the repository level as compared to the single-level case. The *3DEC* analyses further indicate that all of the multi-level layouts considered cause destressed zones extending in depth well beyond that induced by a single-level layout.

A *3DEC* model with altered properties at the repository region was analyzed to evaluate the influence from the excavation openings in the repository. The results show that extent and depth of the tensile yield near the ground surface and fracture zone displacements are very similar for the model with equivalent properties for the repository region and the model with uniform properties. It seems, therefore, that the thermo-mechanical effects of excavation openings on a global scale are not significant. However, the level of detail in the models in this study does not allow for any discussion in details on stresses and strains close to the repository excavations.

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DETERMINATION OF IN-SITU FRACTURE APERTURES FROM DIGITAL BOREHOLE IMAGES

Maria C. Johansson Engineering Geology, KTH, SE-10044 STOCKHOLM

O. Stephansson Engineering Geology, KTH, SE-10044 STOCKHOLM

Abstract

Imaging methods applied to borehole investigations have become common for mapping and characterisation of the rock mass. Today we have access to detailed information about the rock, but we lack some methods for analysis.

In this study we develop methodology for measurements of in-situ fracture geometry, from optical borehole images (BIP-system). We focus on the detailed information about fracture geometry, available thanks to the high image resolution. We have decided to perform the measurements using digital image processing, to avoid bias from the human analyst, and we present on-going work on the image processing methodology.

Our method is based on iterative intensity thresholding. We work on grey-scale images, of open fractures that fully intersect the borehole. The fracture trace comes out as a dark sinusoidal in the borehole image.

First, the darkest pixels in the image are extracted. Then the pixels, which are immediate neighbours to the first set, are included, under the condition that they are darker than a somewhat lower threshold. The including of neighbours is repeated until the fracture trace is filled.

The resulting sinusoidal fracture trace is then used for finding an approximation of the fracture plane (Method of Least Squares). The fracture plane orientation is used for determination of true aperture from the apparent fracture seen in the image. After this, fracture aperture statistics can be determined.

The method works well for images of open fractures of simple geometry (sine wave). It needs to be improved to handle more complex geometry, e.g. crossing fracture traces. Today, some minor interaction from the analyst is needed, but slight modifications will minimise this.

1 Introduction

Imaging methods applied to borehole investigations have become common for mapping and characterisation of the rock mass. Technical development of logging equipment has made it possible to increase the resolution in the images, and also to increase the speed of logging. This has led to a situation where we have access to detailed information about the rock, but we lack methods for detailed analysis.

In this study we develop methodology for measurements of in-situ fracture geometry, from optical borehole images, registred with the Borehole Image Processing System (BIPS). This kind of analysis is often restricted to the determination of fracture frequency, and fracture plane orientation, but we instead focus on the detailed information about fracture geometry, that is available thanks to the high image resolution.

In order to make our method work without severe bias from the human analyst, we have introduced digital image processing into our work. With digital image processing, we refer to computerised image analysis, where various algorithms are applied on the digital image to automatically extract and measure some feature of interest. This can be with more or less input from the analyst. (The advantage with automatic analysis, compared to manual, is that measurements become more objective and can be repeated by others. On the other hand, the disadvantage is that much of the human analyst's knowledge is hard to convey to a computer).

Two main branches of special interest for this study are found in the literature. They are: 1) image analysis for determination of detailed fracture geometry and 2) application of image processing on images of the rock mass in-situ, and in particular, on borehole images. In the first group, there is a study closely related to our project (Hakami, 1995). In this work the focus is measurements of fracture aperture distribution. One method developed for this is an image analysis methodology applied on microscopy images of a fracture filled with fluorescence resin. In the second group, which deals with in-situ images, interesting contributions are the attempts to perform automatic analysis of fractures plane orientation (Hall et al, 1996, Thapa et al 1997) and also the automatic mapping of fractures on a rock face (Reid & Harrison, 1996).

Our objective is to analyse the statistical distribution of fracture aperture for in-situ fractures, but we also hope to reveal how this is related to different fracture sets and their orientation. In this paper we present on-going work, which include an image processing methodology for identification and segmentation of sinusoidal fracture traces in borehole images, and also the determination of fracture plane orientation from those traces.

2 Method and Material

2.1 Digital images

A digital image consists of square image elements, pixels, representing the intensity response of an area of the depicted object. For a colour image, the response is registered for each of the three wave length bands: red, green and blue, while for a grey-scale image, only the intensity is registered. Colour images are easily converted to a "black and white",

grey-scale image, but since this conversion destroys the colour information, the process is not reversible. Another feature of importance is the image resolution, which is typically much lower for a digital image than for a conventional photographic image.

2.2 Image material

The images used in this study are recorded in boreholes at Äspö HRL, using the Borehole Image Processing System (BIPS). The image logging performed with this system result in optical, colour images, covering the whole circumference of the borehole. Since the image is built up from single pixel rows, the maximum image length is (virtually) not limited. The image resolution in depth direction is variable between 0.25, 0.5 and 1 mm/pixel. (The finest resolution applies to images presented in this paper). The circumferencial resolution is fixed at 1 pixel /degree.

2.3 Image processing algorithms

The very first operation that we apply to the image, is a conversion from colour to greyscale. This means a simplification of the image handling, and it is possible to do since we have restricted the study to open fractures. The open fractures appear as dark traces in the image, and for the analysis of those, we need only to utilise the intensity information.



Figure 2-1 BIPS image from borehole KLX02, Äspö HRL (depth 317 m), converted to grey-scale. The resolution is 0.25 mm/pixel in the depth direction and 1 degre/ pixel across the borehole (Ø 76 mm)

Image processing methods for grey-scale images are generally designed to use the pixel intensity in various ways. Either directly, as with intensity thresholding, or indirectly, like in edge detection methods, where it is the changes in intensity between neighbouring pixels that are of interest.

As mentioned, the trace of an open fracture will typically come out as a dark trace in a optical borehole image. After the conversion to grey-scale, we therefore applied intensity thresholding to the grey-scale image. Practically, this means that a binary image (0-1 instead of 0-255) is created, by setting pixels, darker than some threshold value T, to zero. Pixels that are brighter than T, are set to one.

To find an appropriate threshold can be difficult, and we chose not to use a fixed, but instead a dynamic, threshold (which means it is related to some image property, in our case the intensity histogram). We also decided to use a very low threshold for a first segmentation, in order to avoid including the medium-dark pixels, which are dark mineral grains. Some fracture pixels are also medium-dark, and they are included later, by stepwise increase of the threshold value, under the restriction that they must be immediate neighbours to the pixels, that were segmented out in the first step. The algorithm reads like following:

1) In the first segmentation, the darkest 1 % of the pixels of an image, I, is extracted, by choosing a threshold, T_1 , based on the image intensity histogram. In Figure 2-2 we see the resulting image, $T_1(I)$. We also see that almost all of the extracted pixels lie in the fracture.

2) As a consequence of the low threshold in step 1, many of the fracture pixels were not included. The second step was therefore to iteratively increase the threshold $(T_2, T_3, ..., T_n)$, to include more and more pixels.

3) In order to only include those pixels that were neighbours to the first set, $T_1(I)$, an operation called dilation was applied to $T_1(I)$. This operation means that all neighbours to selected pixels in $T_1(I)$ is added to $T_1(I)$, resulting in a new set $D(T_1(I))$, see Figure 2-2 b.

4) The fracture pixels derived with the second threshold, T_2 was then combined with $D(T_1(I))$, using the logical (Boolean) operator AND.

The sequence 2-4 was repeated until the neighbours of outliers started to be included (in this case, five repetitions). The algorithm was then terminated manually. The resulting image, R, is shown in Figure 2-2 c.

2.3 Fracture plane orientation

The fracture plane is then determined from the image pixels in R, by first transforming the pixels back to the location on a cylindrical surface representing the borehole wall, and then fitting a plane through these points (or pixels). The fitting is made as a Method of Least Square fitting (MLS) of two variables; Z=Z(x,y), where $x=r*\cos(\varphi)$ and $y=r*\sin(\varphi)$, where r is the borehole radius, and φ is the angle of rotation around the borehole axis (0-360 degrees, see Figure 2-1).

In Figure 2-3, the intersection between the resulting fracture plane, and the cylinder representing the borehole wall, is plotted on top of the original image, where it constitute a sine curve. The orientation of the fracture plane is determined from the amplitude and phase of the curve, by algebraic manipulation. The resulting parameters are the dip, and dip direction of the plane, relative to the borehole axis.



c)

Figure 2-2 a) The fracture image after one iteration of the thresholding algorithm. b) The dilation of the image in 2-2a. c) The final fracture trace image.



Figure 2-3 The trace of the approximative fracture plane (white trace), on top of the original grey-scale image.

2.4 Fracture aperture

To determine the fracture aperture, we now only have to measure the height of the trace for each column in R (apparent aperture), and calculate the true aperture as the component of the height, that is normal to the fracture plane. The aperture is plotted against orientation in Figure 2-4 a. The fracture aperture distribution can be represented by a histogram (Figure 2-4 b), but later on in our work, this will be more thoroughly analysed, e.g. with respect to



Figure 2-4 a) The fracture apertures measured for the fracture trace in Fig 2-2 c.b) Corresponding histogram for the apertures (n=number of observations).

orientation.

3 Results and discussion

Since this method is still under development, the results are not yet ready. Worth to mention is at least the identification and delineation of sinusoidal fracture traces, that worked well for the small number of images that we have analysed so far. The resulting fracture traces seems to be in close agreement to what human vision would identify as the fracture. (This will later be measured in a comparison between automatic delineation and manual digitalisation of the fracture edges).

An observation that we have made is that the images show high variability in various aspects, such as fracture frequency, intersecting and branching fractures, filled and open fractures, rock matrix and also noise. This is caused by the geological variations and sometimes also due technical factors during the logging. To deal with such large variability, is hard, using an automatic method. It would probably require far greater effort of development than is possible in this project. We will therefore focus on handling some delimited parts automatically, but the analyst will at least have to make some intelligent work by choosing what algorithms to use on a specific image. Two of the cases we consider to work with are:

- more complex trace geometry, e.g. traces that are crossing each other

- mineral filled fractures

To work with mineral filled fractures would require modifications. Fractures containing white fillings can be treated in a similarly way as the dark fractures, by creating a negative image, where white fractures come out as dark. In order to distinguish coloured fillings, one will have to work with colour images, since the trace would else appear grey in a grey-scale image, and therefore be hard to segment out from the surrounding wall, particularly when the segmentation is based on intensity thresholdning.

Regarding the aperture measurements, one has to remember that image processing applied in this way, is an attempt to measure the 3D reality in a 2D image. We can not easily determine where pieces of rock have fallen out and left a cavity, which we might regard as natural aperture. Since we are also determining the fracture trace from various levels of grey, and sometimes have to decide where in visual appearance of a diffuse fracture edge is located, we can not treat the measured values as exact measurements. To do this we have to adjust the measures to other observations and performed some type of calibrating measurements. Until we do that we will treat the apertures as relative measurements, and compare them to each other, in order to look for features that vary with orientation of the fracture plane.

In our opinion, it is clear that image processing has strengths as a method of analysis for borehole images. The major benefit is that image processing makes the measurements become more objective and consistent. The analyst or a colleague analyst will also be able to repeat the measurements. We therefore believe that image processing will become an important tool for analysis of the in-situ rock mass, and that it should at least be utilised for research. The more common application of image processing in other fields, e.g. medicine and also remote sensing, also shows the potential of image processing applied to borehole images, since many of the problems encountered and solved in those fields are very similar to the problems seen in our application.

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THE IDENTIFICATION OF POTENTIAL FLOWING FEATURES FOR A CONCEPTUAL MODEL OF FRACTURE FLOW AT SELLAFIELD

P.J. Degnan¹, A.E. Milodowski² and S. Todman³ ¹United Kingdom Nirex Limited, ² British Geological Survey, ³ AEA Technology For correspondence E-mail: Paul Degnan@nirex.co.uk, Fax Number: UK 1235-825 367

ABSTRACT

United Kingdom Nirex Limited (Nirex) has studied in detail the geology and hydrogeology at a site near Sellafield in Cumbria, NW England to determine the suitability, or otherwise, of the site as the location for a deep repository for intermediate-level and certain low-level radioactive wastes. A key factor in determining site suitability is the nature of groundwater flow in the repository host rock: the Borrowdale Volcanic Group. In the host rock, flow takes place predominantly through a limited subset of discontinuities, mainly fractures, parts of which form networks of connected channels. Within this overall understanding of the nature of groundwater flow, there is a wide range of possible geometries for the flow channels. Determination of the applicable conceptualisation of the flow system must be soundly based on site characterisation data as a prerequisite for any numerical modelling study. In this presentation, a brief description of aspects of the core characterisation studies which were used to identify the location, orientation and mineralogical characteristics of the particular discontinuities referred to as Potential Flowing Features (PFFs) is provided. These features have either demonstrable present day open porosity or display evidence of groundwater flow as part of the evolution of the current groundwater system. The PFF information has been integrated with data derived from hydraulic testing to provide the basis for robust conceptual models, which have been used in a performance assessment of the site [1].

INTRODUCTION

The safe disposal of radioactive waste is a problem common to many developed and technologically emerging countries. The waste arises from a diverse number of processes, such as spent nuclear fuel and the disposal of various radioactive sources used in medical and industrial applications. In Britain, Nirex is the organisation charged by the government with the responsibility for the management and disposal of intermediate-level and certain low-level radioactive wastes.

Since 1989, Nirex has been investigating the geology and hydrogeology of a site near Sellafield in NW England to determine whether it might be suitable for the construction of an underground disposal facility (a repository) for radioactive waste¹. An intensive programme of site characterisation provided the site specific data necessary for a series of performance assessments to investigate the long-term safety of the disposal measures proposed. The performance assessments consider the total system (inventory together with near-field, geosphere and biosphere processes) in order to derive risks to compare against regulatory targets. An important component of that system is the groundwater pathway through the geosphere. The poster to accompany this text concentrates on the methods that have been applied to identify the nature of the groundwater pathways through the host rock, the Borrowdale Volcanic Group, and the conceptualisation of those pathways for incorporation into numerical models for groundwater flow.

¹ In March 1997 Nirex was refused planning permission to build a proposed underground rock laboratory at Sellafield. Since that time Nirex has concentrated on consolidating the information gained from the Sellafield investigations and making it available to interested parties.

GEOLOGY

The Sellafield area is in a transitional structural zone between the western margin of the Lake District Massif of Lower Palaeozoic crystalline rocks and the adjacent, mainly offshore, East Irish Sea Basin of younger sedimentary rocks. Major structural elements include east-north-easterly trending faults and faults trending between north and north west. These faults influenced sedimentary basin development, for example, the Fleming Hall Fault Zone locally formed the eastern edge of Permian evaporites and other basinal facies.

In the Sellafield area, the Ordovician age Borrowdale Volcanic Group was considered as the host rock for the potential underground repository. The group comprises a several kilometre thick sequence of volcanic and volcaniclastic rocks, including lavas, ignimbrites, welded and non-welded tuffs, breccias and intrusive igneous rocks. The whole assemblage has been metamorphosed at low (sub-greenschist) grade. The unconformity surface with the younger sedimentary rocks dips gently (ca. 25 degrees) to the west and is down-faulted in that direction, such that at the coast it is some 1,600m below the ground surface. In the area of the potential repository the top surface of the Borrowdale Volcanic Group is at a depth of approximately 500m below ground level, beneath the immediately overlying Brockram, a sedimentary breccia of Permian age. This is, in turn, overlain by early Triassic sandstones of the Sherwood Sandstone Group. Quaternary deposits up to 180m thick occur offshore, and thicknesses up to 100m are present onshore. The Quaternary sediments are sedimentologically heterogeneous, comprising glacial tills and glaciotectonised sands and gravels that are laterally variable.

THE IDENTIFICATION OF POTENTIAL FLOWING FEATURES

Because of the igneous and metamorphic history of the Borrowdale Volcanic Group, the rock matrix is inherently of low permeability and most of the groundwater flow takes place through open discontinuities. Faulting is pervasive in the Borrowdale Volcanic Group and affects the rock properties. A variety of other geological discontinuities that could be associated with groundwater flow have been recognised including open joints, altered intrusive (sill and dyke) margins, lithological boundaries, internal disconformities and mineralised fractures and vuggy veins of several ages.

In the deep (to 2 km) boreholes drilled by Nirex at Sellafield, a comprehensive dataset of discontinuities was compiled from geophysical wireline logging results (especially resistivity and sonic) and from core analysis. Examination of the spatial distribution of the total fracture dataset (visual appraisal of the data and statistical interpretations) indicates that they can be sub-divided into discrete borehole intervals (structural domains), which have a common set of discontinuity characteristics, namely fracture frequency and orientation. Although strongly controlled by lithology, the structural domains have a general association with other features, such as faults.

The discontinuities relevant to groundwater flow modelling comprise fractures which are capable of carrying groundwater on time scales relevant to safety assessment, which can be beyond a million years. Potential Flowing Features (PFFs) have been defined as a subset of the total discontinuity dataset on the basis of mineralogical and/or petrographical characteristics, as discontinuities or discrete horizons in the rock mass that are capable of conducting groundwater flow at the present day. They :

- have demonstrable open porosity, at least at core scale;
- display evidence of mineralisation or rock water interaction that can be attributed directly to the development of the present day groundwater system.

Dating of the late calcite mineralisation partially infilling the fractures, using a whole crystal ²³⁰Th/²³⁴U technique, indicates ages from 17,000 to greater than 300,000 years BP (Before Present). However, the coeval association of the late calcite cements with a Fe and Mn oxyhydroxide mineralisation episode, which has been dated as being Tertiary (Miocene) and possibly up to the present day, indicates that the calcite mineralisation phase may extend from the late Tertiary up to the present time.

PFFs have been recognised in all lithological units that have undergone mineralogical logging and partial correlations with other parameters and features have been noted (e.g. fault damage zones, disconformities, palaeo-weathering horizons). A definitive summary dataset of PFFs was created and applied in the latest performance assessment [1]. As part of that assessment, a visual inspection of PFF clusters compared against flow zones suggested good correlation. This relationship was used to augment the PFF dataset, which at the time of Nirex 97 did not extend over the entire length of all boreholes.

THE CONCEPTUALISATION OF FLOWING FEATURES

Flow in the Borrowdale Volcanic Group is believed to be through a sparse network of interconnected open fractures and the recognition of the significance of PFFs for flow represents a major development in understanding. At the location in the borehole where they are observed, PFFs are considered to indicate the presence of a Flowing Feature (FF) within the local unobserved rock volume. Measurements of the frequency and orientation of PFFs have been used as the basis for describing the large-scale pattern of flow through Flowing Feature clusters in the Borrowdale Volcanic Group as PFFs identified in a borehole are considered to correspond to the FFs at the location of the borehole. This is supported by the following observations. The presence of the late calcite suggests that the PFFs have carried groundwater relevant to the current groundwater system. Borehole flow zone characterisation studies have shown that there is a correlation between the location of inflows into the boreholes and the PFFs. An analysis of the results of Short Interval Tests (hydraulic) which were carried out on short intervals of borehole (about 1.5m long) showed that:

- For intervals not crossed by an identified PFF, the effective permeability determined from the tests is consistent with the permeability of the matrix in the Borrowdale Volcanic Group (determined from measurements on cores).
- For intervals crossed by one or more identified PFFs, the effective permeability is significantly larger on average than that of the matrix.

The concept that flow in the Borrowdale Volcanic Group is through a subset of the total fracture network is consistent with interpretations of the data from the large scale (3 month) Borehole RCF3 Pump Test undertaken by Nirex. A conclusion of that test was that on a length scale of less than hundreds of metres from the source (that is, the test interval) the groundwater flow through the Borrowdale Volcanic Group is controlled by the interconnection of many features of comparatively low transmissivity, as opposed to a smaller number of features with high transmissivities.

The PFFs in the Borrowdale Volcanic Group do not appear to have a simple random distribution in space, but instead show marked spatial clustering. **[H]** illustrates the clustering directly. It shows how the density of PFFs varies down the logged intervals of Borehole 2 (note that mineralogical logging has not been undertaken between approximately -1100 and -1500 maOD in Borehole 2). The density at each point was calculated from the number of PFFs in a 10m interval centred on the point. Pronounced clusters are clearly present.

Figure 1 shows the clustering more indirectly. It presents a comparison of the distribution of the density of PFFs with that to be expected from a Poisson (random) distribution in space. The figure

shows a histogram of the frequencies of 10 metre intervals containing different numbers of PFFs for the observed PFFs and the corresponding histogram for a Poisson distribution (with the same total number of features). Only sections of borehole longer than 100m long that had been logged for PFFs were included in the analysis. Logged intervals of smaller length that had been targeted on specific features of interest were excluded from the analysis. This was done to avoid biasing the analysis. It can be seen that there are many more sections of borehole crossed by a very small number of PFFs, and fewer sections of borehole with many PFFs, than would be expected for a Poisson distribution.

Clustering of PFFs appears to be significant hydrogeologically. Analysis of the Environmental Pressure Measurement hydraulic tests (length scale of ca. 50m) indicates that the effective permeabilities for intervals containing, or inferred to contain, PFF clusters are generally larger than the effective permeabilities for intervals not containing PFF clusters, although there is some overlap between the distributions. Furthermore, the results of the Fracture Network hydraulic tests, which were carried out on intervals of borehole about 20m long, also appear to suggest that clustering of PFFs is important, in that the effective permeability for intervals crossed by many PFFs is higher than might be expected given the number of PFFs crossing the interval and the permeability of intervals crossed by one PFF.

In the Nirex 97 performance assessment [1], the conceptual model for flow in the Borrowdale Volcanic Group adopted was that the flow is through a network of FFs, which correspond in boreholes to PFFs where these have been logged, and that the FFs exhibit, at least locally, clustering, which is significant hydrogeologically. However, the connectivity of the FF clusters, which is an important aspect of the conceptual model, cannot be determined from the borehole samples. Alternative concepts are possible (Figure 2). At one extreme, the FF clusters (and indeed, the PFF clusters upon which they are based) might simply be isolated regions with a higher local density of FFs, connected to each other by a relatively sparse network of background FFs. At the other end of the spectrum, the FF clusters might form a well-connected network of one-dimensional 'strings' or two-dimensional 'sheets'. The hydrogeological properties of the Borrowdale Volcanic Group might be expected to be quite different for the case in which the FF clusters form a wellconnected network, and the case in which they do not. The extent, significance (in terms of transmissivity) and the orientations of the components in such a network may well vary with time in response to several processes, for example, changes in regional or local stress fields and mineral dissolution and precipitation. One possible model for FF connectivity is illustrated in Figure 3. In order to address the uncertainty about the connectivity of FF clusters within the Borrowdale Volcanic Group, two extreme conceptual models were analysed in the upscaling calculations to derive effective regional-scale [1].

The advance in understanding gained from the appreciation of the significance of PFFs provides a firm foundation for models in which the groundwater flow in the Borrowdale Volcanic Group is modelled as being through a network of discrete features. In particular, it means that the density of the features in question and the distribution of their orientation can be quantified with less uncertainty than has hitherto been the case.

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