5 EVALUATION OF MODELS FOR GROUNDWATER FLOW

5.1 INTRODUCTION

The purpose of the hydrogeological model of Äspö is to provide a condensed description of hydrogeological features as they are interpreted to exist today. The model is based on the geological model of Äspö and a number of concepts used for the evaluation of the hydraulic properties of the rock mass. The geological model is an important base for the interpretation of the data forming the hydrogeological model. The hydrogeological model can first of all be used for understanding observations and the underlying hydraulic systems. It is also the base for setting up numerical groundwater flow models, which are used for calculations of water pressure distribution, fluxes in the rock mass and flow paths.

The hydrogeological model of the Äspö area consists of two main concepts for describing the domains of the rock mass; hydraulic conductor domains (called water-bearing zones in *Gustafson et al /1991/*) and hydraulic rock mass domains (see *Table 5-1* and *Figure 5-1*). Groundwater flow modelling has mainly been based on a stochastic continuum approach. The hydrogeological concepts are presented in detail in *Rhén et al /1997b/* together with the hydrogeological model of Äspö. The groundwater flow is dependent on the salinity as this affects the density of the water and, thus, the hydraulic forces. The effects of the salinity could have been discussed in this chapter, but as the salinity is also considered to be a natural tracer the concepts and results are presented in *Chapter 7, Transport of solutes.*

Pre-investigation methods

A number of pre-investigation methods were used to describe the hydrogeological model. These are briefly outlined below.

Compilation of basic information on the hydrological condition of the area around Äspö, such as the extent of drainage basins, flow rates in rivers, precipitation, location of peatlands, etc. was performed by the Swedish Meteorological and Hydrological Institute (SMHI). No new measurement stations were established as available data were considered sufficient for the objectives for the project.

Table 5-1. Condensed description of the groundwater flow model of the Äspö site used within the Äspö HRL Project up to 1995.

GROUNDWATER FLOW MODEL OF THE ÄSPÖ SITE
Stochastic continuum model

Scope
Natural groundwater flow, flow to laboratory tunnel

Process description
Continuity equation (mass balance equation).
Equation of motion (Darcy's law, including density-driven flow).
Equation of state (Salinity-density relationships).

CONCEPTS

Geometrical framework and parameters
Three-dimensional box divided into:

- Hydraulic conductor domains. 2-D features (location, extent, orientation).
- Hydraulic rock mass domains. 3-D features (location of boundaries).

Material properties
Hydraulic conductor domains: Transmissivity (T).
Hydraulic rock mass domains: Hydraulic conductivity (K).

Spatial assignment method
T: Deterministic assignment.
K : log-normal distributions for hydraulic conductivity (K_g, $s(\mathrm{Log}_{10}(K))$.
K and s are dependent on the cell size within a domain in the numerical model.

Boundary conditions
Upper: fixed infiltration rate on Äspö, constant head at sea and peat areas.
Lower: no flow.
Side: prescribed pressure (hydrostatic).
Salinity: prescribed initial conditions, linear increase with depth at vertical boundaries (see concepts for the transport of solutes).
Tunnel: hydraulic resistance (skin factor) around the tunnel and prescribed pressure (atmospheric) **or** flow rate into the tunnel.

Numerical tools
Finite-volume code PHOENICS.

Output parameters
Groundwater pressure
Groundwater flux

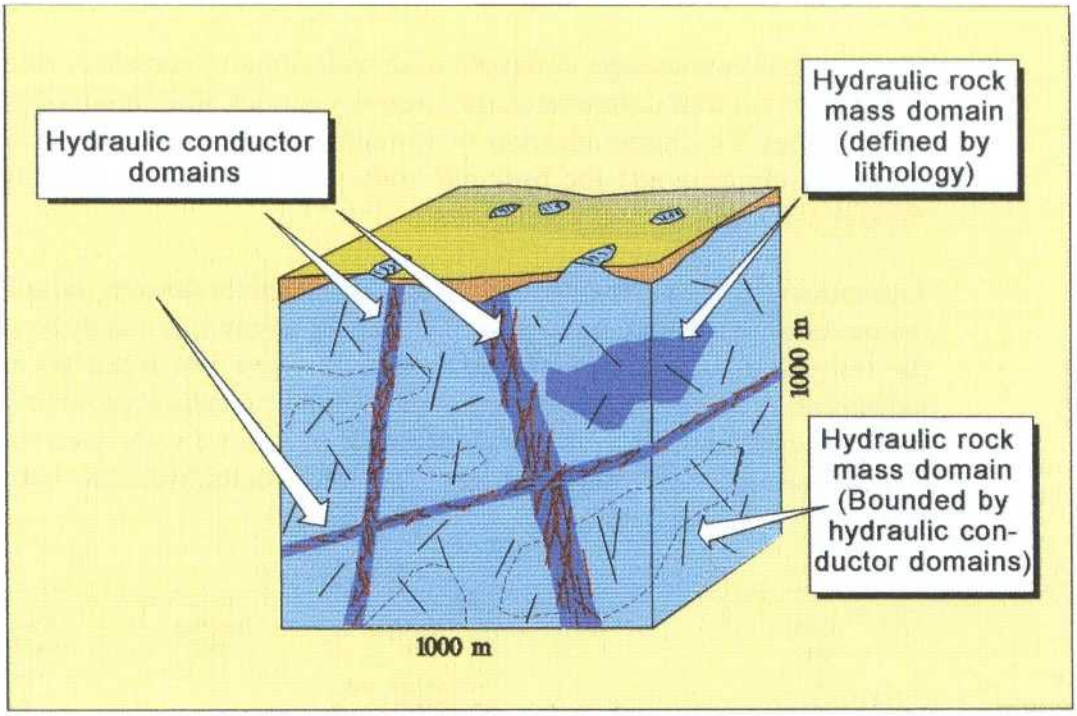


Figure 5-1. Schematic description of two main hydrogeological concepts. Hydraulic conductor domains: 2-D features (location, extent, orientation) and hydraulic rock mass domains: 3-D features.

The hydraulic properties of the hydraulic conductor domains and the hydraulic rock mass domains were characterized by means of a number of different hydraulic tests:

- airlift pumping of percussion drilled boreholes and 100 m sections of core drilled boreholes,
- pump testing and cleaning of borehole (performed directly after drilling),
- flow-meter logging,
- injection tests (packer spacing 3 or 30 m),
- interference tests,
- dilution tests,
- monitoring of water pressure in the rock-mass.

Long-term monitoring was also performed during the pre-investigation phase.

The hydrogeological description of the rock was derived from the evaluated hydraulic parameters together with the geological model. The first three methods were performed more or less systematically in all cored boreholes. The percussion drilled boreholes were either tested by airlift pumping or using a submersible pump. About 100 pumping tests were performed with test sections exceeding 100 m. Injection tests with a packer spacing of 3 m (about 1200 tests, injection and recovery periods about 10 + 10 minutes) were performed in 8 cored boreholes and injection tests with a packer spacing of 30 m (65 tests, injection and recovery periods about 2 h + 2 h) were conducted in 3 cored boreholes. Roughly 20 interference tests were performed, generally with a pumping period of 3 days and pressure recovery period of 2 days. Two long interference tests were also performed, with pumping periods of about 60 and 30 days but with somewhat shorter recovery periods. The pre-investigation methodology for characterization of hydraulic properties of the hydraulic conductor domains and the hydraulic rock mass domains is presented in *Figures 5-2* to *5-4*.

Transmissivity was assigned to each hydraulic conductor domain, included in the model as a deterministic feature. The transmissivity was mainly based on the test results but in a few cases a value was assigned based on expert judgement, as no test was performed in the hydraulic conductor domain. Data from the injection tests, with a packer spacing of 3 m, were analysed statistically to provide estimates of the hydraulic properties of the hydraulic rock mass domains.

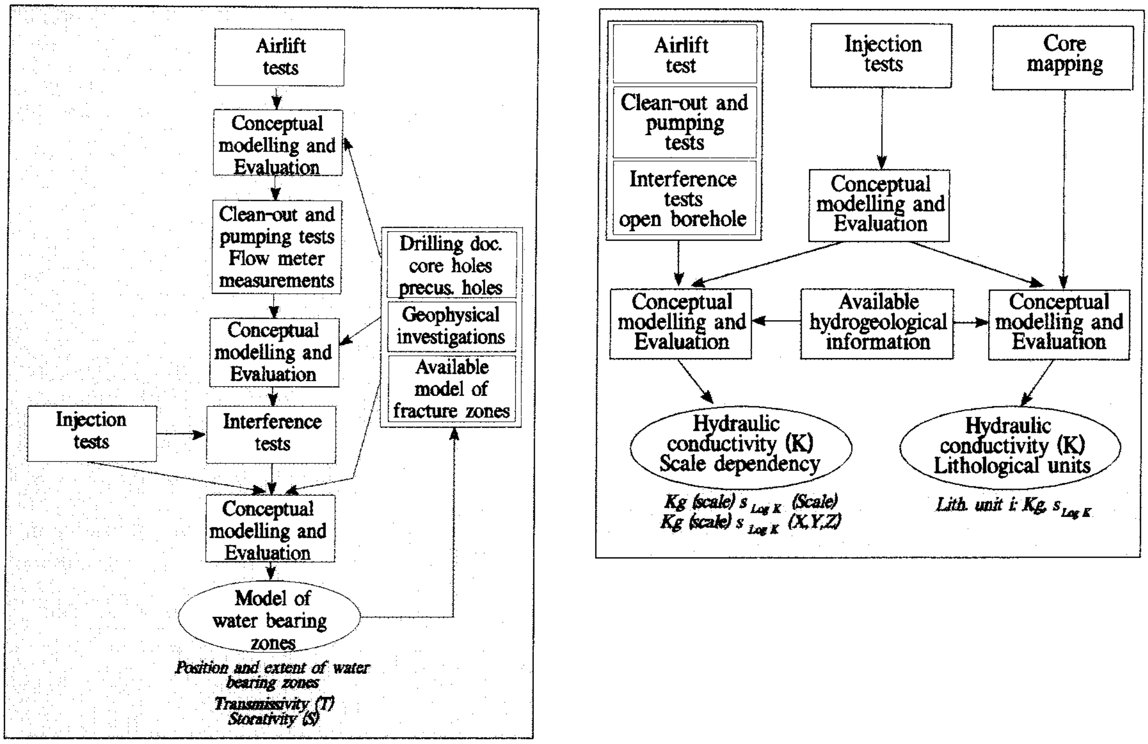


Figure 5-2. *Pre-investigation methodology. Left: Properties of hydraulic conductor domains (or Water-bearing zones). Right: Properties of hydraulic rock mass domains. Tests to different scales (tested borehole section length and test time) provide empirical relations for scale dependency of hydraulic conductivity.* K_g*: geometric mean hydraulic conductivity.* s_{logK} *: standard deviation of* $Log_{10}K$*.*

Investigation methods used during construction

The hydraulic data collected during the construction were mainly:

- pressure build-up tests (single-hole test),
- interference test (tunnel boreholes used as sinks),

- dilution test (surface boreholes),
- monitoring of water pressure in the rock-mass,
- flow-meter logging or logging by inflow observation during drilling,
- observation of pressure responses in monitored boreholes during drilling of core holes,
- mapping of water-conducting and grouted fractures in the tunnel,
- measuring the water flow into the tunnel.

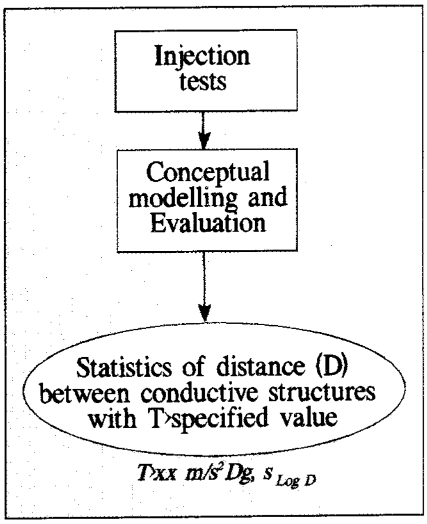


***Figure 5-3**. Pre-investigation methodology. Block scale. Statistics of distance between conductive features. The 1-D approach is used by studying the distance (D) between conductive features, with a transmissivity (T) greater than a specified value along boreholes. The characteristic values evaluated for the distribution is the geometric mean distance (Dg) and the standard deviation of* $Log_{10}D$ (s_{LogD}).

The main purpose was to obtain data for comparison with the predictions. Data were compiled for 150-m long tunnel sections */Markström and Erlström, 1996/.*

To some extent water will flow into a tunnel when the tunnel is excavated below the groundwater level. At the outset of the Äspö HRL project it was decided that a more or less tight tunnel was not needed and that grouting should be limited and controlled in order to limit disturbance of the chemical composition of the groundwater. It was also of interest to obtain sufficiently large inflows to obtain clear responses in the observation boreholes around the tunnel. Hence, the excavation itself could be seen as a very long-term hydraulic test which could be used to;

- check the structural model by observing where and when drawdown occurred and also how great the drawdown was, and

- check and calibrate groundwater flow models.

A summarized evaluation, based on data from a comparison between prediction and outcome */Rhén et al, 1997a/* is presented in this chapter.

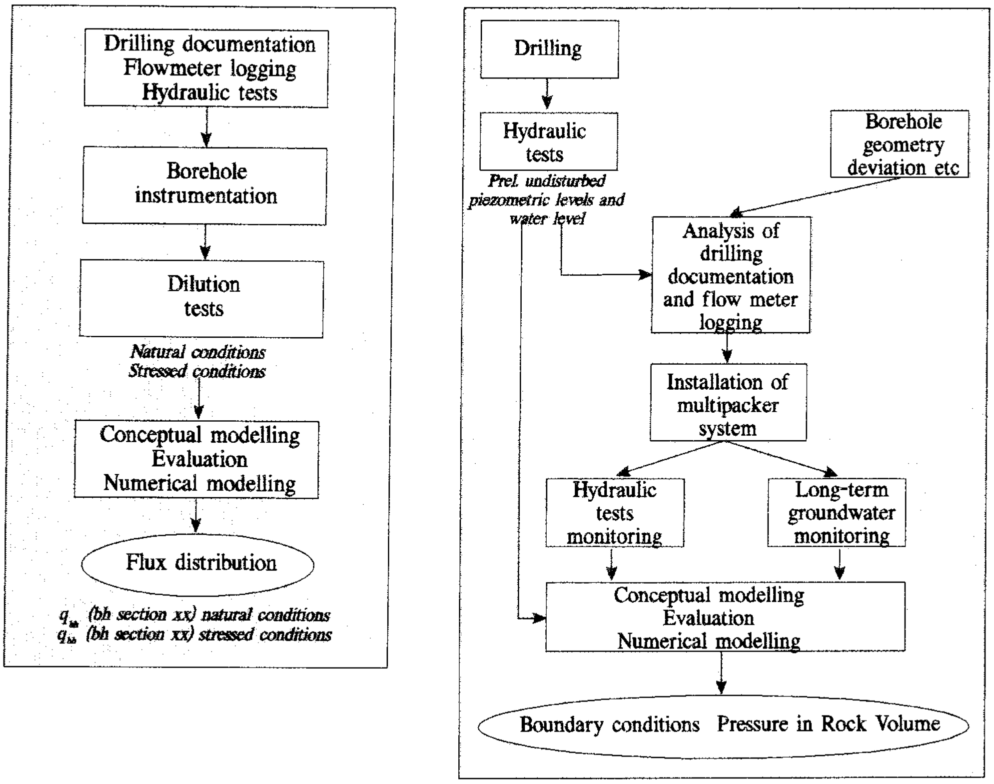


Figure 5-4. *Pre-investigation methodology. Left: Flux distribution in the rock mass. The dilution test gives the flow rate through the borehole section. Right: Boundary conditions and pressure in the rock mass. Pressure measurements are the base for assessing suitable initial and boundary conditions in groundwater flow models.*

Method of evaluating hydraulic properties

Transmissivity (T): T for a section in a borehole is generally evaluated from transient tests using the method developed by *Cooper and Jacob /1946/*, and is valid for the test section or hydraulic conductor interpreted to control the measured pressure change. If it has only been possible to evaluate the specific capacity (Q/s), the transmissivity is estimated as T= f(Q/s), where the function f(Q/s) is the linear least-square-fit of $\mathrm{Log}_{10}(T)$ versus $\mathrm{Log}_{10}(Q/s)$ for tests with evaluated T and similar test length and test time. The rationale for this is that Q/s is roughly proportional to T */Carlsson and Gustafson, 1984, Domenico and Schwartz, 1990/*. If T is evaluated for the entire borehole (T_{tot}) and flow logging has been done, the approximate T distribution along the borehole is estimated according to *Earlougher /1977/* as $T_i = T_{tot} \cdot dQ_i / Q_{tot}$, where Q_{tot} is the total flow rate and dQ_i is the flow rate change per length L_i. The dynamic viscosity of the fluid and fluid density was assumed to be approximately constant within the rock volume tested.

The evaluated T for hydraulic conductor domains is normally based on a transient test where the feature has been straddled by packers. If there were no tests where the hydraulic conductor domain was straddled by packers, T_i (defined as above) was used for the feature. If no test at all had been performed in a geologically defined fracture zone, the geological character, properties of other hydraulic conductor domains and expert judgement were used to estimate possible properties.

Hydraulic conductivity (K): It is assumed that the medium is a stochastic continuum and a local K, in the text called *effective hydraulic conductivity*, is generally evaluated as T/L, where L is the test section length, also here in the text called *test scale*. Evaluated K is always linked to the test scale in the approach used. It will be discussed further in the text below.

The rationale for using a 2-D approach for the evaluation of the hydraulic tests is that in most cases the flow-dimension can be interpreted to be radial flow.

The evaluated transmissivities for the hydraulic conductor domains were adjusted by calibration of a numerical groundwater flow model made in 1990 */Wikberg et al, 1991/*. The adjustments were fairly small.

Hydrogeological model 1996

Figure 5-5 shows the hydrogeological model of the hydraulic conductor domains and the hydraulic rock mass domains after the construction phase. A detailed description of the model is presented in *Rhén et al /1997b/* and the model will also be discussed in the sections that follow.

5.2 GEOMETRICAL FRAMEWORK

The model comprises the following geometrical concepts:

- hydraulic conductor domains,
- hydraulic rock mass domains.

Hydraulic conductor domains are large two-dimensional features with hydraulic properties different from the surrounding rock. They are generally defined geologically as major discontinuities but in some cases they may mainly be defined by interpretation of results from hydraulic interference testing.

Hydraulic rock mass domains are geometrically defined volumes in space with properties different from surrounding domains (rock mass and conductors).

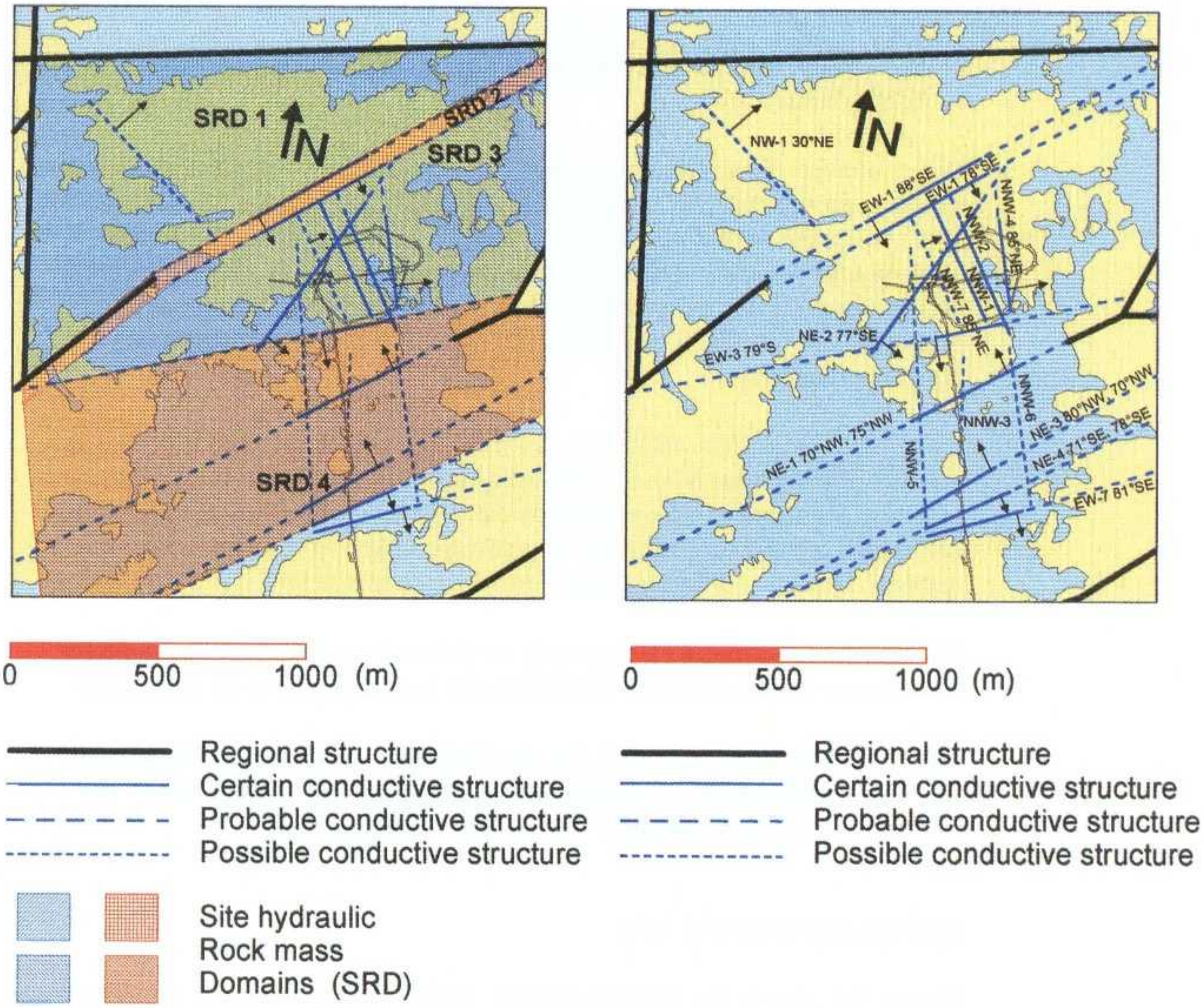


Figure 5-5. *Model 96 of the hydraulic rock mass domains and hydraulic conductor domains /Rhén et al, 1997b/.*

They may either be defined by lithological domains or purely by interpretation of results from hydraulic tests.

Hydraulic conductor domains

The most important hydraulic conductor domains were approximately at predicted positions. The domains checked were the ones that intersected the tunnel or were expected to be close to the tunnel. The volume checked was thus limited but it can also be noted that **no** unexpected hydraulic conductor domains with large transmissivities were found along the tunnel! A few corrections of other domains were also made based on re-interpretation of the data. *Figure 5-7* shows the hydraulic conductor domains according to predictions and according to the new model. Most of the hydraulic conductor domains correspond to the major fracture zones shown in *Chapter 3* but some

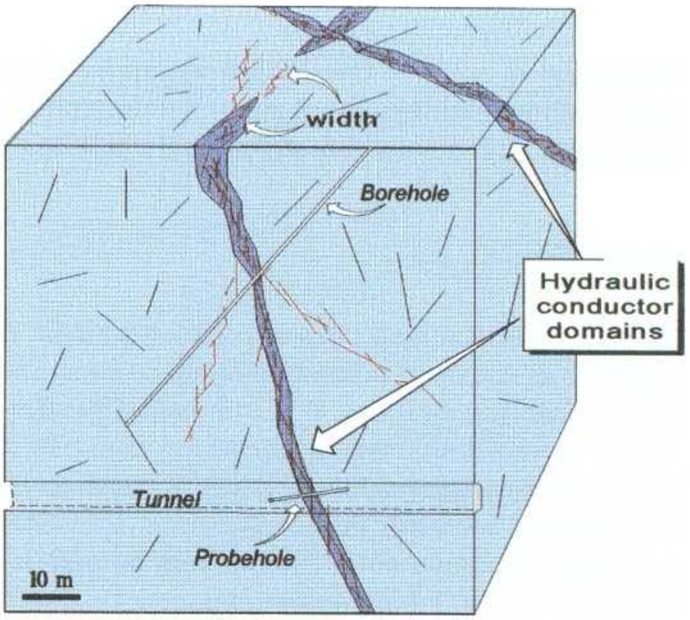


Figure 5-6. *Schematic description of hydraulic conductor domains and test methods used during the pre-investigation and construction phases.*

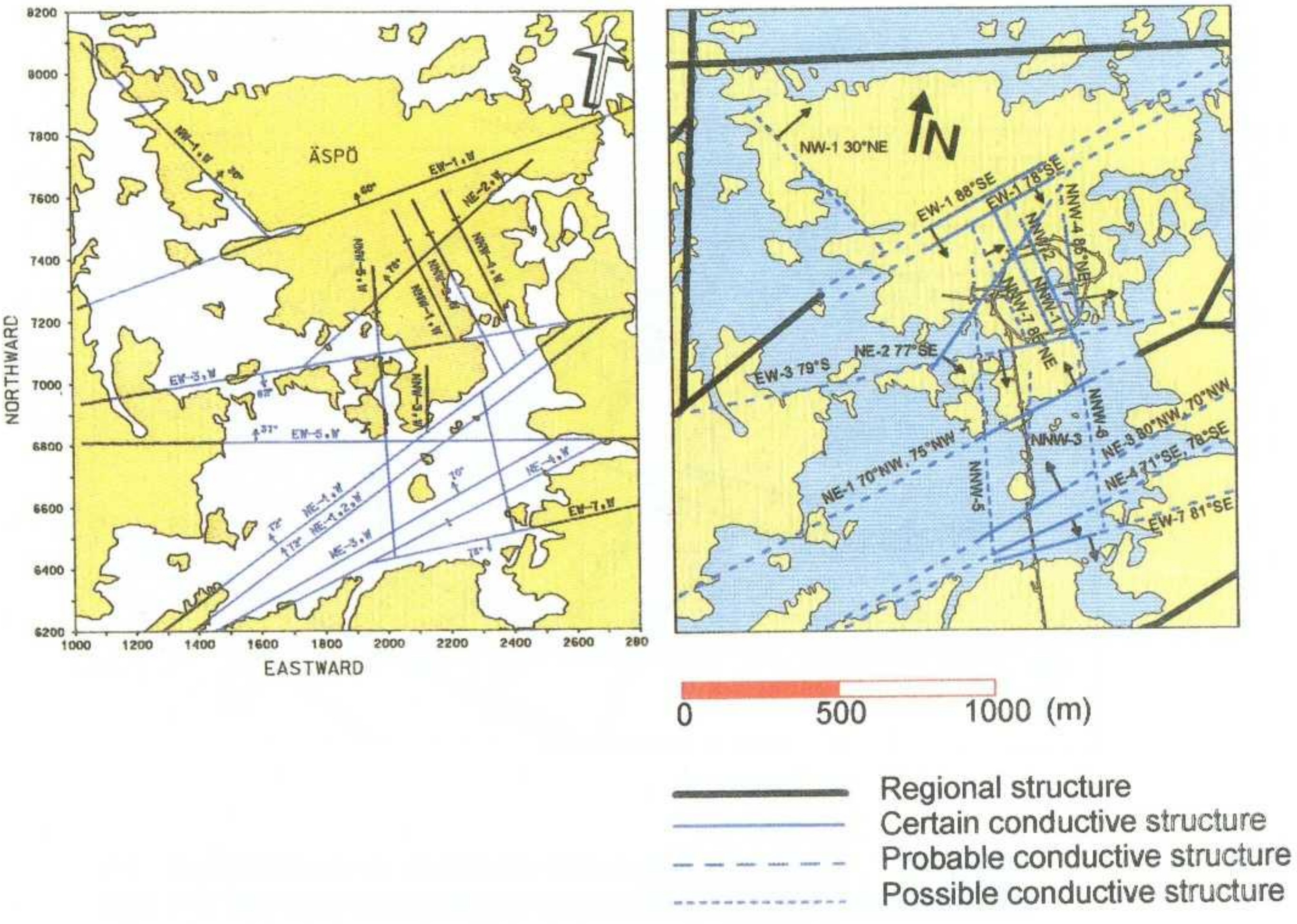


Figure 5-7. *Left: Model 1990 of hydraulic conductors from the pre-investigation phase - site scale. /Gustafson et al 1991/. Right: 1996 model of hydraulic conductors - site scale /Rhén et al, 1997b/.*

correspond to what in that chapter are called fracture swarms. Hydraulic conductor domains NNW-1,2 and 7 are interpreted as consisting of steeply dipping fractures mainly with strikes N-S and WNW to NW (see *Figure 5-8).*

Identification

Identification of a water-bearing zone (hydraulic conductor domain) with respect to its existence, position and extent is generally based on geological and geophysical investigations. It is then generally what in *Chapter 3* are called 'major fracture zones' that are identified. However, interference tests may be a very useful complement to the geological and geophysical interpretations of the position and extent of a certain zone. Hydraulic tests must be made to estimate the hydraulic connectivity within the zone and with other zones. Low transmissivity of a zone and/or long distances between observation points and/or few observation points for the pressure responses, however, reduce the chances of confirming a zone with interference tests suggested by geological and geophysical investigations. It is therefore important to have a close interaction with the geological team when new boreholes are planned.

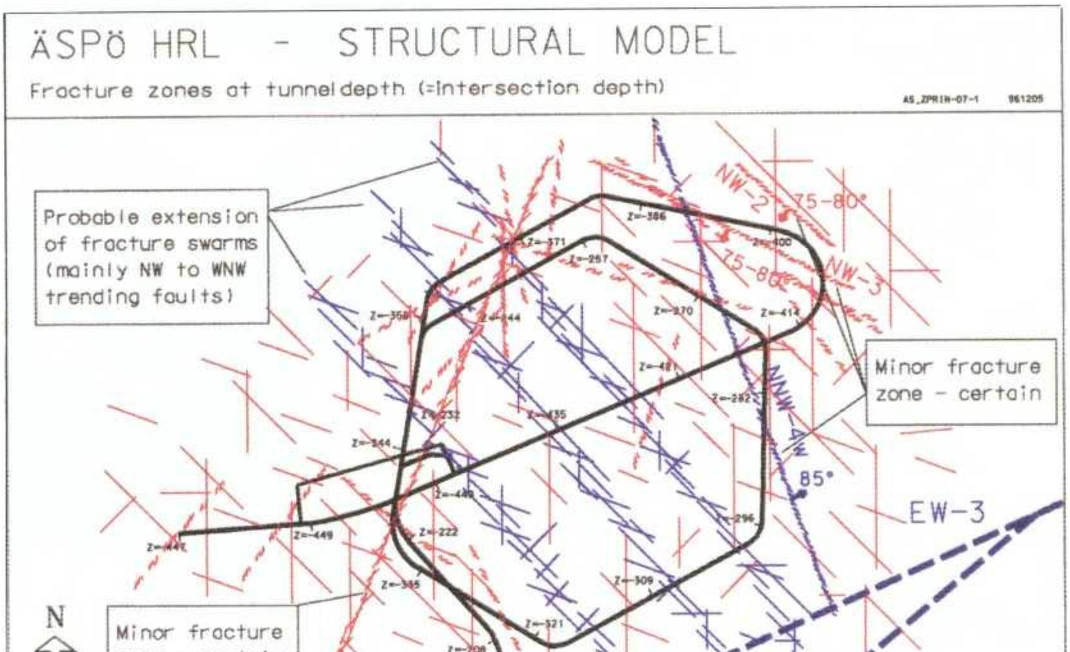


Figure 5-8. *1996 model of hydraulic conductors on southern Äspö - site scale. A schematic figure of the fracture sets present at Äspö and how these sets are interpreted to form some of the hydraulic conductor domains. The domains called NNW-xx are formed by interconnected, steeply dipping fractures mainly with strikes N-S and WNW to NW. The frequency of the WNW to NW fractures dominates (see Chapter 3). (Fracture lengths not to scale.)*

For what are here called fracture swarms (or also minor zones in *Chapter 3*), it is difficult to define the water-bearing zones by means of geological and geophysical investigations, but the position can be indicated from the interpretation of interference test results. The possibility of identification is, however, very dependent on the number of observation boreholes and the way in which they are equipped (number of packed off sections) and their positions in relation to the pumped borehole.

Even though it has not been demonstrated at the Äspö HRL, it should be possible to identify a subhorizontal conductive feature by means of interference testing if several boreholes penetrating the feature within a distance of a few hundred metres and with the boreholes packed off in a proper way. At the Finnsjön site in Sweden a large subhorizontal fracture zone was investigated */Ahlbom and Smellie, 1991/.*

The width of the hydraulic conductor domains must generally be defined in the numerical continuum models. This can only be done approximately as there is no sharp interface between a hydraulic conductor domain and the hydraulic rock mass domain. The width varies also from place to place, as was mentioned in *Chapter 3* and illustrated in *Figure* 5-6. However, this is not such a sensitive factor as the transmissivity evaluated from the hydraulic tests and that also controls the flow in the domain. The width is only used to calculate a hydraulic conductivity for the estimated width.

The Äspö model

The concept of deterministic hydraulic conductor domains was found useful and feasible. The hydraulic conductor domains of importance for Äspö were found at approximately the predicted intersections with the tunnel or at positions close to the tunnel spiral. The numerical groundwater flow modelling shows that the measured hydraulic potential can be described fairly well using the hydraulic conductor domains and their transmissivities given in the descriptive hydrogeological model */Wikberg et al, 1991, Svensson 1991, 1994, 1995b, Gustafson and Ström, 1995/.* Based on the results from the groundwater flow modelling and a re-evaluation of available data a few minor changes were made in the location and properties of the hydraulic conductor domains in 1996. However, the fracture swarms that were given deterministic positions and extents can possibly be modelled as stochastic features in space or by assigning anisotropic material properties to the rock mass where these fracture swarms were defined. More details concerning the groundwater flow modelling are presented in *Section 5.6.*

The pre-investigations were focused on the actual site for the Äspö HRL. Due to this, the extent of the hydraulic conductor domains outside southern Äspö and below about 1000 m depth should be considered uncertain due to the limited investigations. Additional investigations would be needed to provide a better definition of the geometry of the hydraulic conductor domains somewhat outside the rock volume of the facility. However, at some distance from a facility it will be of less importance to know the exact geometry and properties of the hydraulic conductor domains for calculation of the flow field in the rock volume for the facility.

In the cases in which the predictions were less good a number of uncertainties were reported, but still the features were judged to be deterministic because several indications pointed in the same direction. An example is the sub-horizontal domain EW-5, which was considered as a possible zone in the 1990 model but was excluded from the 1996 model (see *Rhén et al /1997a/* for details).

Hydraulic rock mass domains

Several investigations in Sweden and Finland indicate that the rock becomes less permeable with depth */Ahlbom et al, 1991a, 1991b, 1992a, 1992b, Rhén and Gustafson, 1990* and *Öhberg et al, 1994/.* Rock down to a depth of 100 or 200 m has an effective hydraulic conductivity (K) 100-1000 times greater than the effective K for the depth 500-1500 m according to the regression lines in the reports.

At the four SKB study sites there are hardly any low-conductivity borehole sections down to 100-200 m depth, but below this depth a large number were recorded as being at the lower measurement limit */Ahlbom et al, 1991a, 1991b, 1992a, 1992b/* (see examples in *Figure 5-9).* The hydraulic conductivity is definitely lower below 100 to 200 m compared with above, but the suggested decrease based on a power function can be discussed. From an examination of the plots it is not obvious that there is a clear decrease below 100-200 m. A similar conclusion is drawn in *Winberg /1989/.* In that report it is concluded that there is mainly a variation with depth around a constant mean value for the hydraulic conductivity below 200 m depth at the sites Gideå, Fjällveden and Kamlunge.

For three of the sites (Gideå, Fjällveden and Kamlunge) the fracture frequency is 4-5.5/m down to 100 to 200 m and 2-2.5/m below 200 m at two sites and below 500 m at one site (Gideå). The fracture frequency is fairly constant below the depths mentioned above. The rock types at these three sites are mainly sedimentary gneiss (Fjällveden and Gideå) or a mixture of sedimentary gneiss and granite (Kamlunge). The fourth site is dominated by Småland granite (Klipperås) .

At the Äspö HRL the decrease in K with depth is not so clear (see *Figures 5-10--5-12).* On Äspö K is fairly constant down to 600 m, and below that, data were only obtained from only one subvertical corehole (KAS02). Below 600 m there are relatively few measurements but the tests indicate that the effective K is around 20% of the effective K within the depth range of 0-600 m. (All boreholes within the Äspö and in surrounding areas with test scales of approximately 100 m are included, see *Rhén et al, 1997b.*) Taking into account

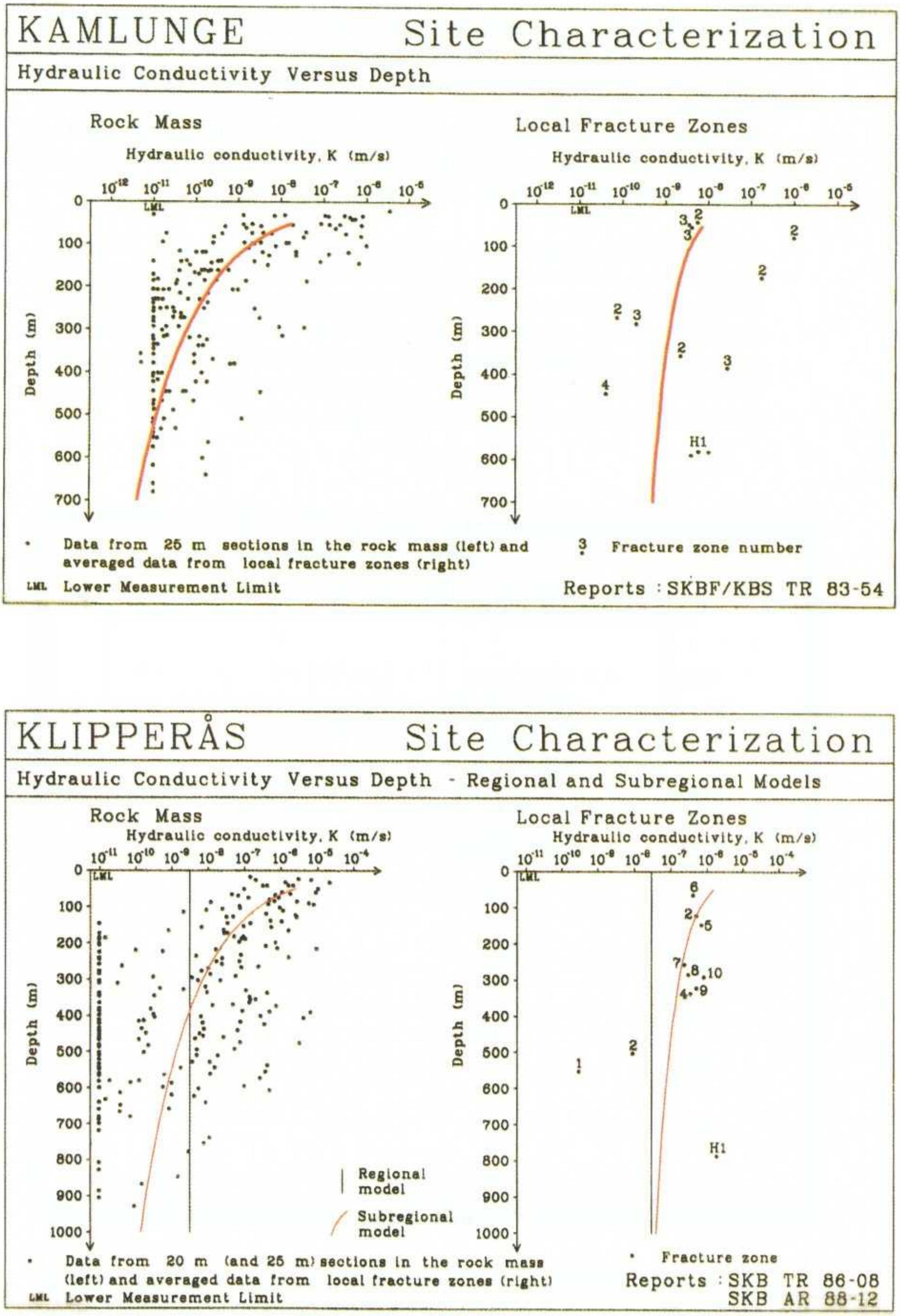


Figure 5-9. *Hydraulic conductivities evaluated Kamlunge (test scale 25 m) and Klipperås (test scales 20 and 25 m) /Ahlbom et al, 1992a, 1992b/.*

the fact that the test scale below 600 m is around 300 m and above about 100 m and also the relations between K and different test scales shown in *Rhén et al/ 1997b/*, the effective K value below 600 m should rather be 10% of the effective K within depth range 0-600 m for test scale 100 m. The base for the conclusion that K does not decrease down to a depth of 600 m is the injection tests with 3 m packer spacing and the hydraulic tests at the 100 m test scale performed at Äspö (see *Figure 5-12) /Rhén et al, 1997b/.*

The mean fracture frequency on southern Äspö is about 3.4/m for 50 m depth intervals down to 400 m depth */Liedholm, 1991a/.* The fracture frequency for the uppermost 100 m is about 4.2/m. At the deepest part of cored boreholes KAS07 and KAS08 (depth about 450-500 m) the fracture frequency increases due to fracture zone NE-1. Below about 700 m the fracture frequency increases in KAS02, possibly because NE-1 is close to the borehole. Thus, there is no clear decrease in fracture frequency with depth at Äspö.

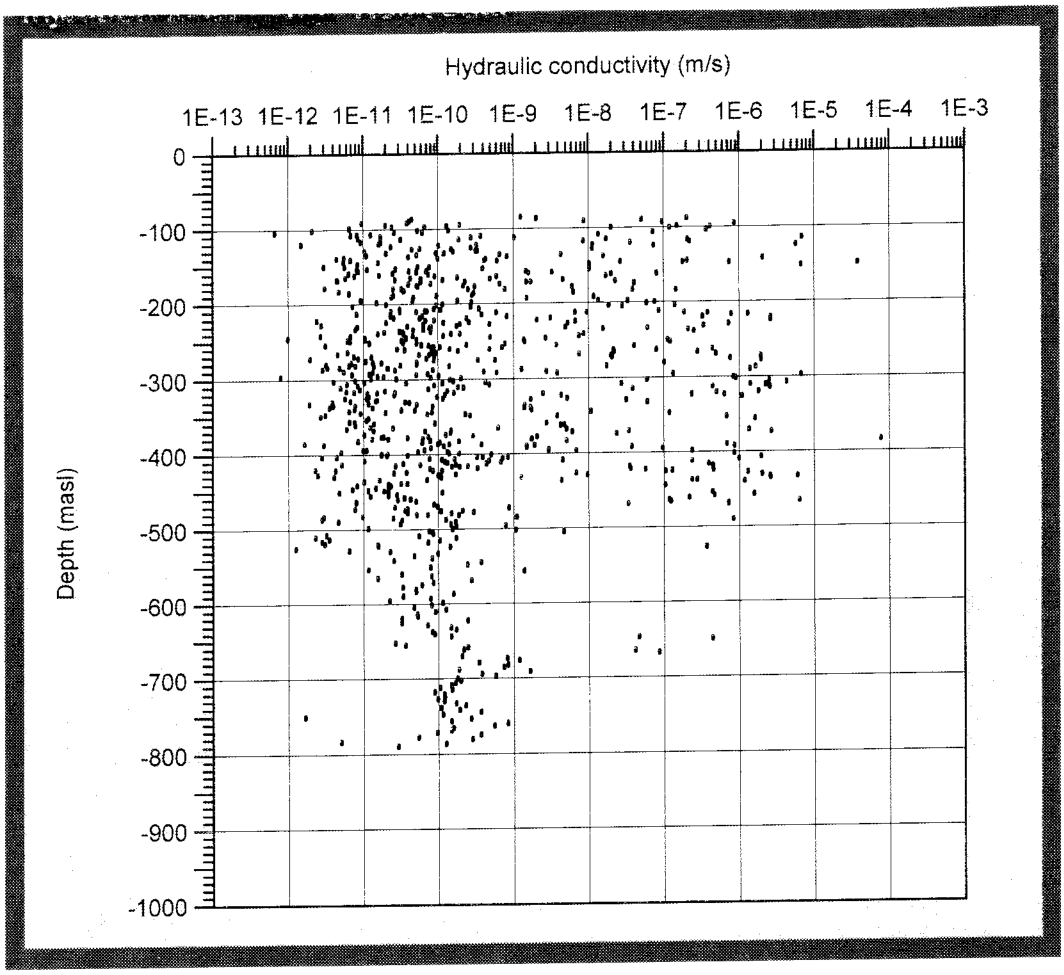


Figure 5-10. *Hydraulic conductivities evaluated for southern Äspö (test scale 3 m) based on data from coreholes KAS02, 05-08. Data for borehole sections which are intersected by the hydraulic conductor domains in Model 96 are excluded in the figure. Data below depth about 525 m is only from one borehole, KAS02.*

In summary, the hydraulic conductivity is fairly constant down to a depth of 500 m at Äspö and below that level there is possibly a decrease according to the pre-investigations. (Exclusion of borehole sections interpreted to be intersected by the deterministic hydraulic conductor domains in the 3 m test scale does not change the conclusion, see *Figure 5-11* and *5-12*). Based on the additional data from the construction phase this conclusion still holds.

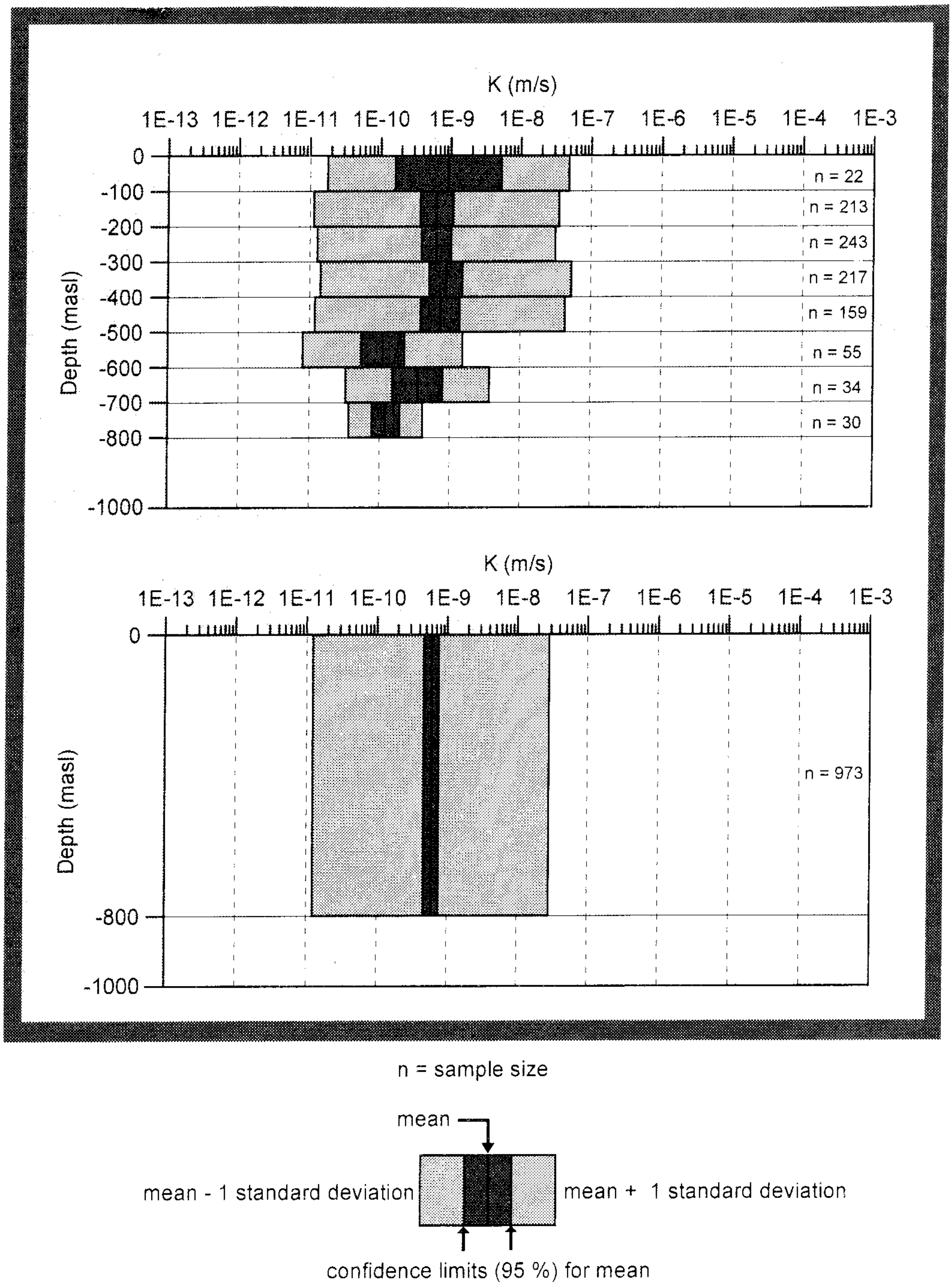


Figure 5-11. *Hydraulic conductivity (K) distribution on the site scale. (mean= arithmetic mean of* Log_{10} *(K), standard deviation=Standard deviation of* Log_{10} *(K), n=sample size). Test scale 3 m. Data from cored boreholes KAS02,05-08 on Äspö. Sample statistics based on the data presented in Figure 5-10.*

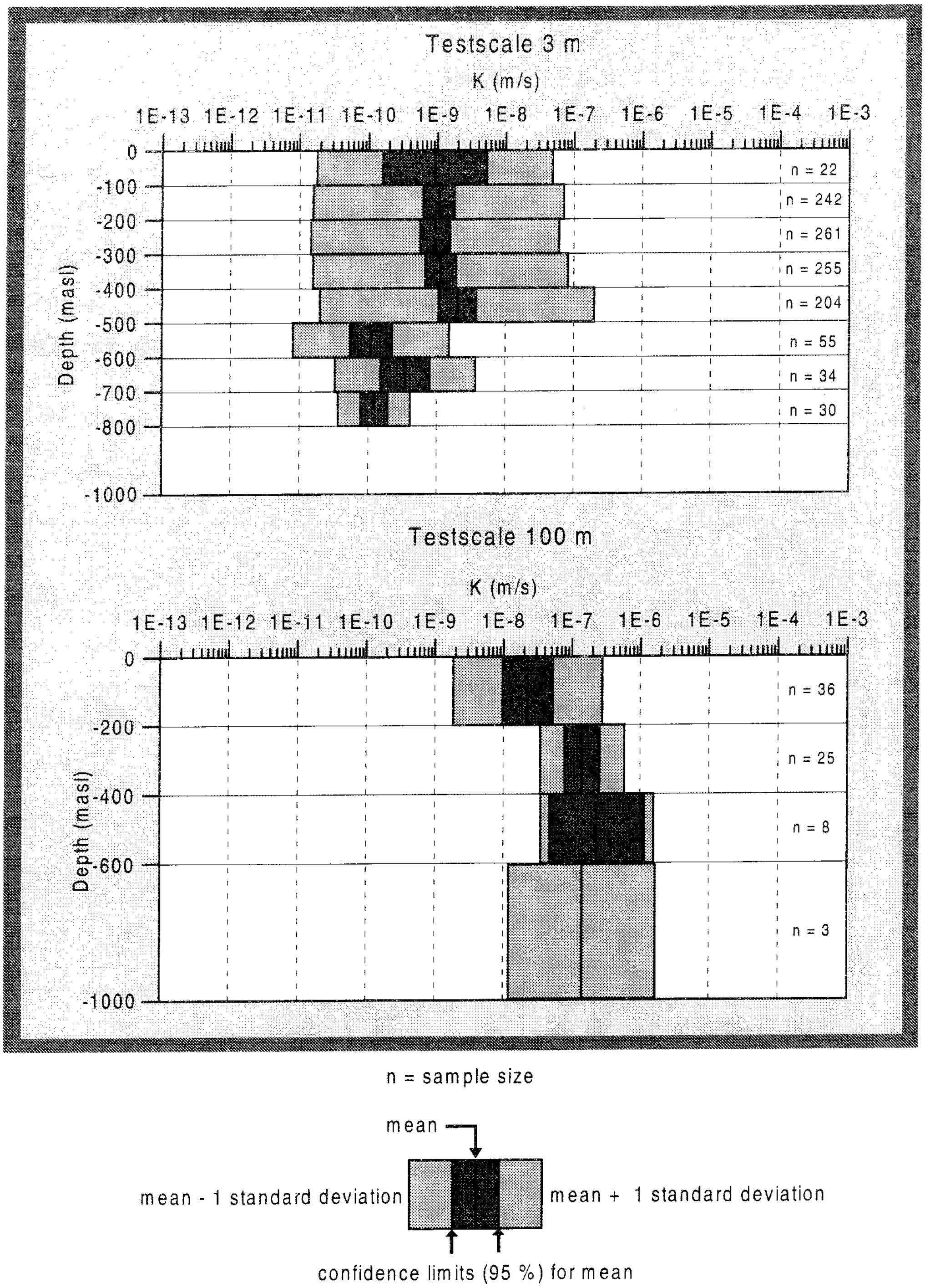


Figure 5-12. *Hydraulic conductivity (K) distribution on the site scale. (mean= arithmetic mean of* $Log_{10}(K)$*, standard deviation=Standard deviation of* $Log_{10}(K)$*, n=sample size). Data for both test scales include all test sections, thus sections interpreted to be hydraulic conductor domains and hydraulic rock mass domains.*

Top: *Test scale 3 m. Sample statistics based on cored boreholes KAS02-08 on Äspö.*

Bottom: *Test scale 100 m. Sample statistics based on tests in cored and percussion-drilled boreholes on Äspö.*

Identification

To characterize the hydraulic properties of the rock mass hydraulic tests must be performed systematically in boreholes. The boreholes must of course penetrate the rock mass in a way that can be expected to provide reliable samples of the rock mass properties. The test scale must be linked to the expected sizes of the lithological units if hydraulic properties are to be determined for these units. In the case of Äspö, greenstone occurs as minor inclusions, irregular, often elongated, bodies and fine-grained granite generally as dikes. The thickness of the bodies or dikes is generally less than a few metres, which indicates that the packer spacing should not be more than a few metres to permit estimation of the properties of the lithological units.

The Äspö model

The Äspö model was divided into three hydraulic rock mass domains in the models for the predictions, northern Äspö, the Äspö shear zone (EW-1) and southern Äspö. It was not possible to check the division into these three domains because the investigations during the construction phase were focused around the tunnel spiral, within the southern Äspö domain, to follow up the predictions made. The 1996 model comprises five domains, northern Äspö, the Äspö shear zone (EW-1), southern Äspö, south of Äspö (see *Figure 5-5*), and a fine-grained granite body at a depth of approximately 300 m within the tunnel spiral.

The Äspö shear zone EW-1 is more conductive than northern Äspö and southern Äspö looking at the single-hole hydraulic tests. However, the interference tests and drawdown during construction of the Äspö HRL showed that EW-1 acts as a semi-permeable boundary The interpretation of this is that there are a number of low-conductivity 'sheets' in the E-W direction within EW-1. These 'sheets' are mainly interpreted to be mylonites lenses found parallel to zone EW-1.

It was found that the rock mass was considerably more conductive south of Äspö than in southern Äspö and as a consequence of this a fourth domain was added to the 1996 model. The borders between the others were changed slightly as the geometry of EW-1 was re-defined based on drillings from the tunnel */Stanfors et al, 1997/*.

At a depth of approximately 300 m within the tunnel spiral there is probably a larger body or number of bodies of fine-grained granite, according to the geological model */Rhén et al, 1997b/*. As the effective hydraulic conductivity is higher compared with other lithological units (see *Figure 5-15*) it is suggested that the volume of the fine-grained granite is a domain (called SDR5 in *Table 5-2*). Based on the results from the simulation with the Bayesian Markov Geostatistical Model (Bay Mar) mentioned in *Rhén et al /1997b/* the domain is approximated to an elliptical body 150 m long with its main axis in the E-W direction. The lengths of the minor axes are estimated to be 0.5 of the main axis length. The centre is estimated to be at a depth of 350 m and in the centre of the spiral. The volume and shape of the domain should be considered uncertain.

5.3 MATERIAL PROPERTIES

The material properties for the domains are

- Hydraulic conductor domain:	Transmissivity (T)
- Hydraulic rock mass domain:	Hydraulic conductivity (K)

T is assumed to be constant and isotropic within a domain and can therefore be described by a single parameter value. K is assumed to be a stochastic property and can vary in space within a hydraulic rock mass domain.

The rationale for having a constant T is that it is generally not possible to determine the variability within a hydraulic conductor domain with the methodology used. First of all the evaluated T generally represents an effective value within a large influence radius. (Evaluation of middle to late time responses.) With this type of evaluation the flow capacity of the domain should be preserved. Early time responses are generally masked by well bore storage and skin effects. Secondly, generally just a few tests have been performed at different locations in a hydraulic conductor domain. The statistics may become poor due to this and correlation models may be difficult or impossible to set up with these data. In the pre-investigation phase it was not considered possible to define the variability within a hydraulic conductor domain.

The variability of the effective hydraulic conductivity is clearly large (see *Figure 5-10).* Instead of estimating a large-scale value for the effective hydraulic conductivity for a rock mass domain the stochastic approach was chosen as it was considered to give a more representative flow distribution in the rock mass. It was also a test to see the importance of the heterogeneity on the undisturbed heads and also the drawdown in numerical groundwater flow simulations.

Transmissivity of hydraulic conductor domains

The predicted ranges of the transmissivities of the most transmissive hydraulic conductor domains were generally within or straddled the range of the geometric mean transmissivity */Rhén et al, 1997a/* (see *Figure 5-13).* The outcome shown in the figure is based on tests performed in boreholes from the surface and from the tunnel.

Parameter estimation

The results show that the variability of the transmissivity within a geologically well defined hydraulic conductor domain is rather large but the predicted

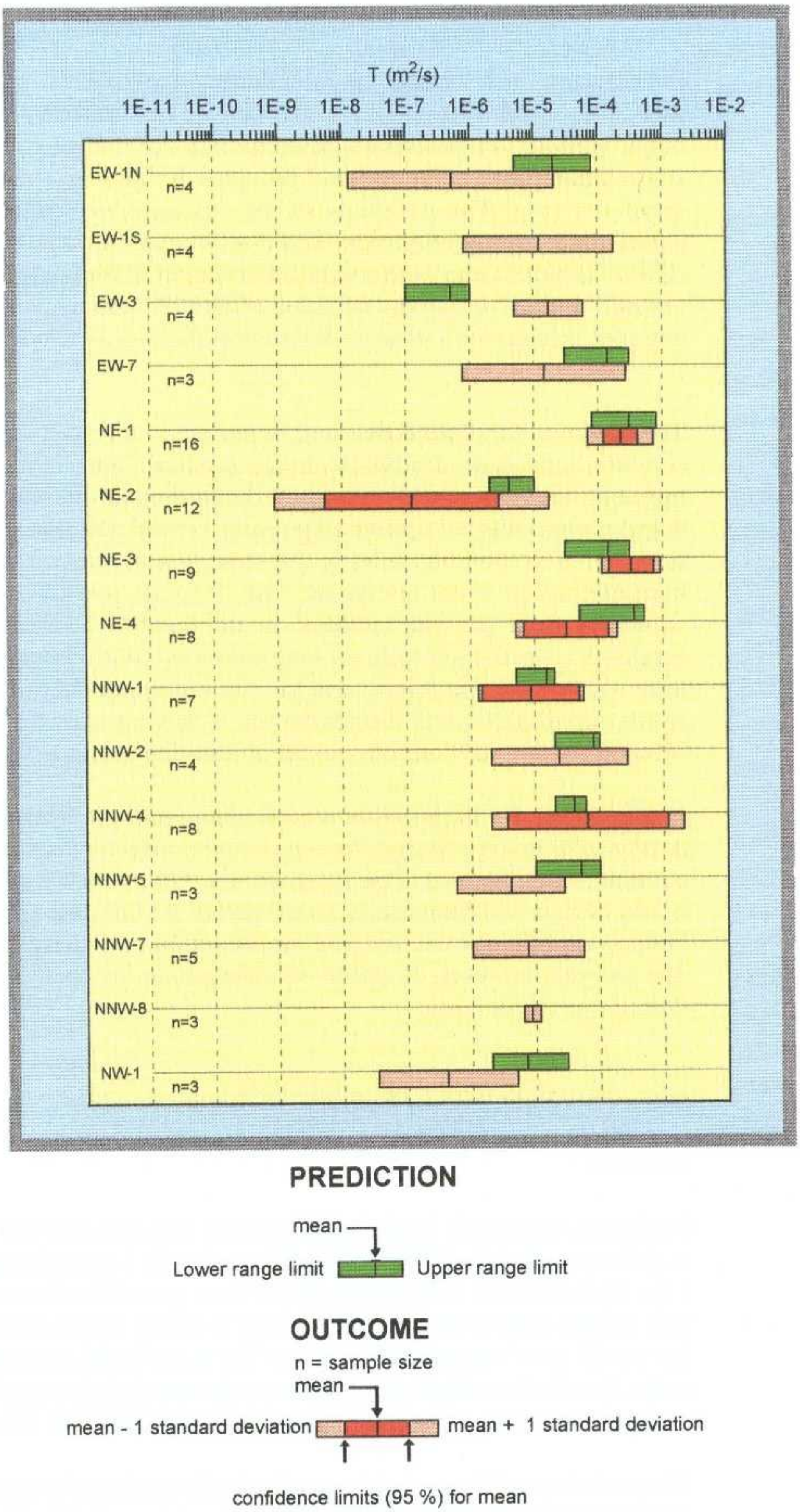


Figure 5-13. *Transmissivity of water-bearing zones for tunnel section 700 - 2875 m. Site scale.(mean = arithmetic mean of Log$_{10}$(T), standard deviation = Standard deviation of Log$_{10}$(T), n = sample size). EW-1S, NNW-7, 8 are new water-bearing zones and NW-1 was re-evaluated.*

ranges for the mean transmissivity (arithmetic mean of the Log_{10}(transmissivity)) are generally within the confidence limits of the mean of the outcome. (The outcome is based on data from the pre-investigation and construction phase.) The standard deviation of the Log_{10}(transmissivity) is about 0.5 to 1. The variability of the transmissivity within a hydraulic conductor domain geologically defined as a fracture swarm or complex zone (EW-1) is rather large, with a standard deviation of the Log_{10}(transmissivity) around 1 to 1.5. The standard deviation of the low-transmissivity feature NE-2, however, is high with a standard deviation of the Log_{10}(transmissivity) around 2.

The transmissivity of the domain can be predicted fairly well if there are a few boreholes through an identified hydraulic conductor domain in which reliable hydraulic tests have been performed. Estimation of the storativity of the domain, which was not a predicted property, is more difficult as it is necessary to have observation boreholes in the same feature rather near the pumped borehole, which is not always the case. It is not possible to evaluate the storativity from the data collected in the pumped borehole, observation boreholes are needed. If there are long distances to the observation boreholes there will be a risk that features that have the same magnitude of transmissivity as the tested feature will disturb the test if they intersect the tested feature between the pumped borehole and the observation borehole, or close by.

It is important for the borehole section intersecting the hydraulic conductor domain to be at some distance from hydraulic conductor domains with higher transmissivities than that of the tested domain. Otherwise it is possible that the nearby domain will dominate the useful part of the transient response, and the evaluation of the test will not give the correct transmissivity for the domain. The test can, however, be useful for interpreting the connectivity between domains on the site scale.

Hydraulic conductivity of hydraulic rock mass domains

Site scale

Predictions were made for the depth intervals 100-200, 200-300 and 300-400 m and were mainly based on the injection tests with 3 m packer spacing. Only a few hydraulic tests in boreholes drilled from ground level were made in the rock volume close to tunnel section 700-1475 during the pre-investigations. A few air-lift tests were performed at the 100 m test scale, but none at smaller scales. Results from Äspö at the 3 m test scale were therefore used as a base for extrapolation for tunnel section 700-1475 m (depth interval 100-200 m).

The predictions of the geometric mean hydraulic conductivity were close to the predicted range for depths of 200-400 m (see *Figure 5-14).* The predictions were outside the range below the Baltic south of Äspö, tunnel section 700-1475 m. The predicted standard deviation was somewhat less than the outcome.

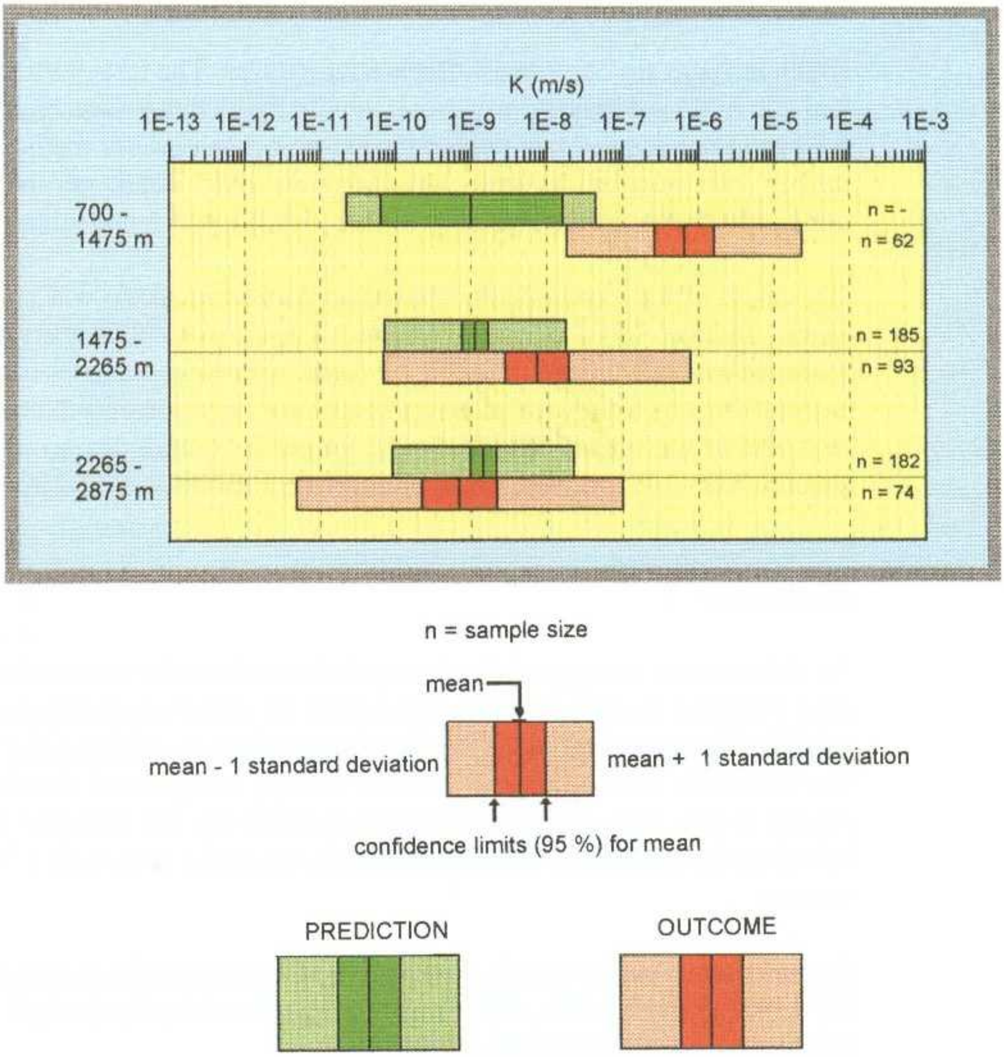


Figure 5-14. *Hydraulic conductivity in tunnel section 700 - 2875 m. Site scale. Test scale 14 m (mean = arithmetic mean of* $Log_{10}(K)$*, standard deviation = Standard deviation of* $Log_{10}(K)$*, n = sample size). Evaluated data comprises both hydraulic rock mass domains and hydraulic conductor domains, but as the number of samples belonging to the latter, the statistics for the rock mass domains are almost identical to the total sample shown here, as shown in Rhén et al /1997b/. It should also be observed that the predicted values were scaled from the 3 m test scale to the 14 m test scale according to the relations suggested in Wikberg et al /1991/. Scaling of test results is discussed in the text below.*
Tunnel section 700 - 1475 m: depth interval 100-200 m.
Tunnel section 1475 - 2265 m: depth interval 200-300 m.
Tunnel section 2265 - 2875 m: depth interval 300-400 m.

The measurements in tunnel section 1475-2875 m seem to indicate a decreasing hydraulic conductivity with depth. However, this is probably due to the large-scale heterogeneity and the anisotropic conditions. Tunnel section 1475-2265 m covers an entire spiral turn but tunnel section 2265-2875 only cover covers two-thirds of a tunnel spiral turn, and thus the anisotropic conditions must affect the result. It is also clear that large-scale heterogeneity can have caused the difference between the two depth intervals, if the individual boreholes on southern Äspö are considered */Rhén et al, 1997a/*. The tests with test scales 3 and 100 m do not indicate any decrease with depth either (see *Figure 5-12*). It is therefore concluded that neither the pre-investigations nor the investigations during construction indicate any decrease with depth of the hydraulic conductivity down to at least 400 m (see also the previous section).

The result of the extrapolation (based on data from Äspö) was poor because tunnel section 700-1475 m penetrated a rock mass that was much more fractured and conductive than that on Äspö, over long stretches of the tunnel. Several fracture zones are intersected that are very transmissive and wide in that part of the tunnel. The hydraulic properties below the sea along tunnel section 700 - 1475 m were thus quite different from those on Äspö.

Äspö model

As a base case it is suggested that no spatial correlation be assumed and that the data used in a stochastic continuum model be scaled according to *Rhén et al /1997b/*. The suggested properties for the populations are shown in *Table 5-2*. The hydraulic conductivity is assumed to have a lognormal distribution (see *Figure 5-21*). The effective hydraulic conductivity for domains SRD1-3 is based on the properties evaluated from the injection tests with a 3 m packer spacing.

As there are no packer tests in domain SRD4 the evaluated properties are based on tests in probe holes, excluding the deterministically defined hydraulic conductors, for tunnel chainage 700-1475 m.

There are no injection tests with a 3 m packer spacing below a depth of about 800 m on southern Äspö, 400 m in the Äspö shear zone and 550 m on northern Äspö, and there is only a limited number of tests below 800 m in the entire area around Äspö. It is therefore suggested that the properties given in the regional model for depths below 600 m be used (see *Chapter 6 in Rhén et al /1997b/*).

Block scale

Two out of six predictions of the geometric mean hydraulic conductivity of 50 m blocks at specified points along the tunnel were within the range. The predicted standard deviation was approximately as the outcome (see *Rhén et al /1997a/*).

Detailed scale

The outcome of the geometric mean hydraulic conductivity for the four lithological units (Småland granite, Äspö diorite, fine-grained granite and greenstone) were close to the predicted ranges (see *Figure 5-15*). The outcome of the difference in hydraulic conductivity between the four lithological units was as predicted. The predicted standard deviation was somewhat less than the outcome.

Table 5-2. Site scale hydraulic Rock mass Domain (SRD) (see *Figure 5-5*). Hydraulic conductivity - Spatial assignment method. d_b = depth to bottom level of numerical model, scale = length of test section, m = arithmetic mean of $Log_{10}(K)$, s = standard deviation of $Log_{10}(K)$.

Group of domains	Depth range (m)	Scale (m)	$m(Log_{10}(K))$ $Log_{10}(m/s)$	$s(Log_{10}(K))$ (-)	Comment
SRD1	0-600	3	-8.74	1.32	KAS03-'rock'
SRD2	0-600	3	-7.82	1.79	KAS04- 'rock'
SRD3	0-600	3	-9.47	1.63	KAS02,05-08-'rock'
SRD4	0-600	15	-6.46	1.61	Probe holes-700-1475 m
SRD1-4	600-d_b	300	-7.33	0.72	Acc. to regional model
SRD5	See text	3	-8.32	1.99	Fine-grained granite

Parameter estimation

The hydraulic conductivity follows approximately a lognormal distribution for test scales longer than about 15 m. For the test scale 3 m the distribution deviates somewhat from the lognormal distribution. The lowest measurable values from the injection tests with packer spacing 3 m were estimated at about 10^{-11} - 10^{-12} m/s, which compares well with the results of tests on the 5 cm scale performed in the Äspö HRL tunnel */Olsson et al, 1996/*.

The temperature has only a minor influence on the evaluated hydraulic properties if the natural temperature gradient (about 15°C per km, */Sundberg, 1991/*) and a depth down to around 1000 m are considered */Rhén et al, 1997a/*. The salinity has even less influence on the viscosity, at least down to a depth of 1000 m at Äspö, as the salinity is less than 2% down to that depth */Rhén et al, 1997b, Earlougher, 1977/*.

The large-scale heterogeneity within a site strongly affects the chances of making reliable estimates of the hydraulic properties using a few boreholes. One reason for the deviations from the Äspö site predictions is the heterogeneity within the site, illustrated by *Figure 5-16*. If a population has a normal distribution it is easy to estimate new sample characteristics if the standard deviation and mean for the sub-samples are known. This is called pooling. To illustrate the uncertainty of the estimated sample statistics in a heterogenous site like Äspö, the sample statistics for each borehole on Äspö (KAS02-08) were used to estimate sample statistics for the Äspö site. Each borehole constitutes a sub-sample with mean = arithmetic mean of $Log_{10}(K)$

and standard deviation = standard deviation of $Log_{10}(K)$ (K= hydraulic conductivity). The variation of the sample statistics can be shown by calculating the sample characteristics for all combinations of 1, 2, 3, 4, 5, 6, and 7 boreholes (see *Figure 5-16*).

As pointed out above, the distribution of $Log_{10}(K)$ for the 3 m scale is not so well described by a normal distribution. In a statistical analysis of the sample based on the original data of the sub-samples the statistics would probably become somewhat different compared with pooling, but a variation of similar magnitude would very probably be seen.

Based on *Figure 5-16* it is concluded that even if the confidence limits for the mean value are narrow for the sample from one or a few boreholes, these limits

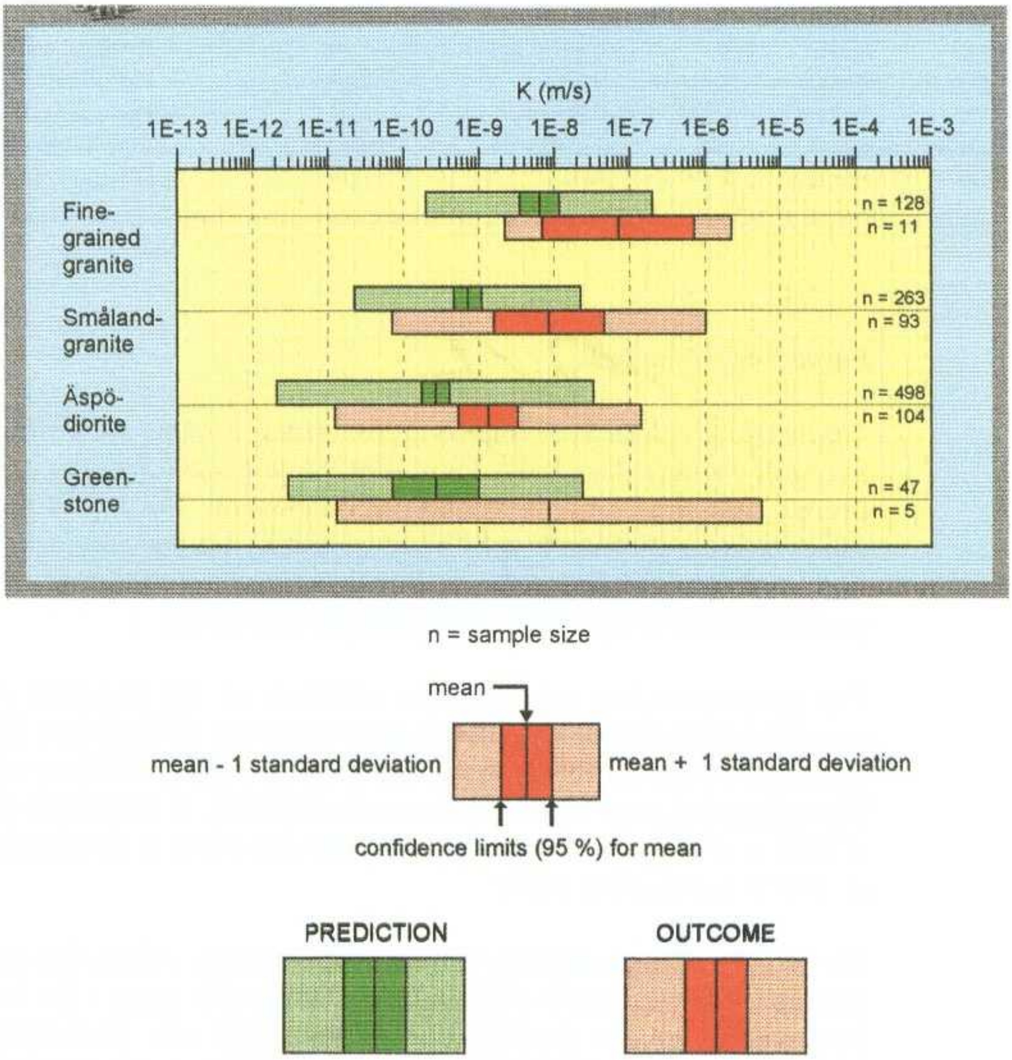


Figure 5-15. *Hydraulic conductivity for different rock types along tunnel section 700 - 2875 m. Detailed scale. Test scale 14 m. The outcome shown is for tunnel section 1475-2875 m except for greenstone, which is for tunnel section 700-2875 m (Fracture zones are included in the outcome.) (mean = arithmetic mean of $Log_{10}(K)$, standard deviation = Standard deviation of $Log_{10}(K)$, n = sample size.)*

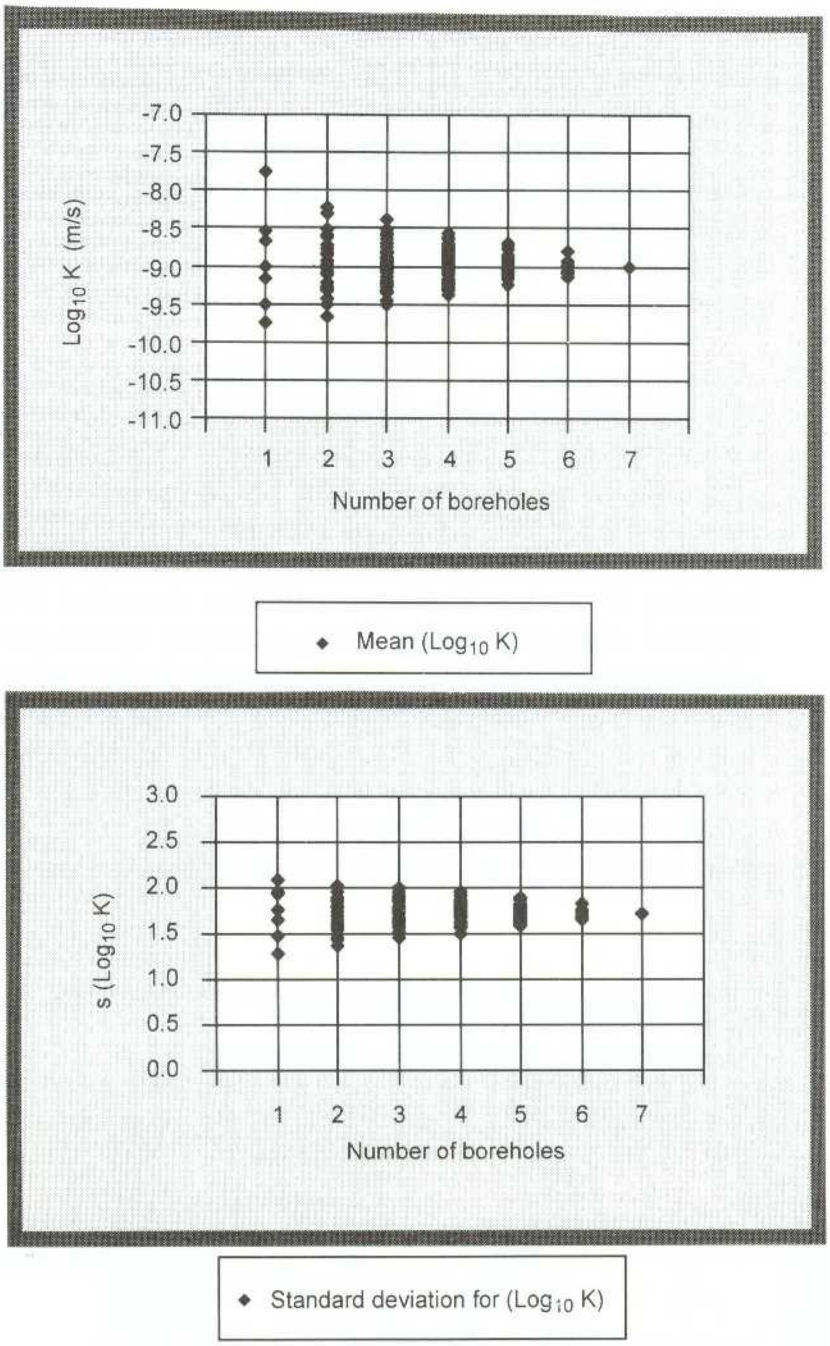


Figure 5-16. *Estimated effective hydraulic conductivity (K) for Äspö, based on the means and standard deviations evaluated for the individual boreholes by pooling under the assumption that $Log_{10}(K)$ on the 3 m test scale has a normal distribution (mean = arithmetic mean of $Log_{10}(K)$, standard deviation = Standard deviation of $Log_{10}(K)$). Each point in the figures above represents estimates of properties based on pooling of data from the number of boreholes shown on the horizontal axis. All possible combinations of boreholes KAS02-08 are shown. (The high value for one borehole and $Log_{10}(K)$ is borehole KAS04.)*

Top: Mean of $Log_{10}(K)$).

Bottom: Standard deviations of $Log_{10}(K)$).

may be irrelevant if the site is heterogenous on a large scale. It is concluded that on a site that is heterogenous on a large scale it is necessary to have more than just a few boreholes to estimate sample characteristics for the entire site. It should, however, be pointed out that the geological model is important both for the investigation strategy and the evaluation of the tests. Understanding of the geological heterogeneity can of course give insight into how to interpret the data and how to assign properties to different domains.

Special consideration in estimating the hydraulic properties of the rock mass domains should be taken in the design of a field programme if anisotropic conditions exist, as illustrated in *Figure 5-17.* The results indicate that at the Äspö site the hydraulic conductivity may be around 100 times greater in the most conductive direction than in the least conductive direction (see *Figure 5-18).* The figure is based on data for tunnel section 1400-3600 m, thus also including the fracture swarms, or as they are also called in this chapter: NNW hydraulic conductor domains. This is essentially a result due to the fact that the main hydraulic conductors on a local scale in the rock mass are fractures trending WNW with high frequency. But as can be seen in *Figure 5-18* the fractures trending N-S are also transmissive. In conclusion there is a need to have boreholes in directions that are not subparallel to find if anisotropic conditions exist. The evaluation methodology of the hydraulic tests may have to be improved for the evaluation of anisotropic conditions.

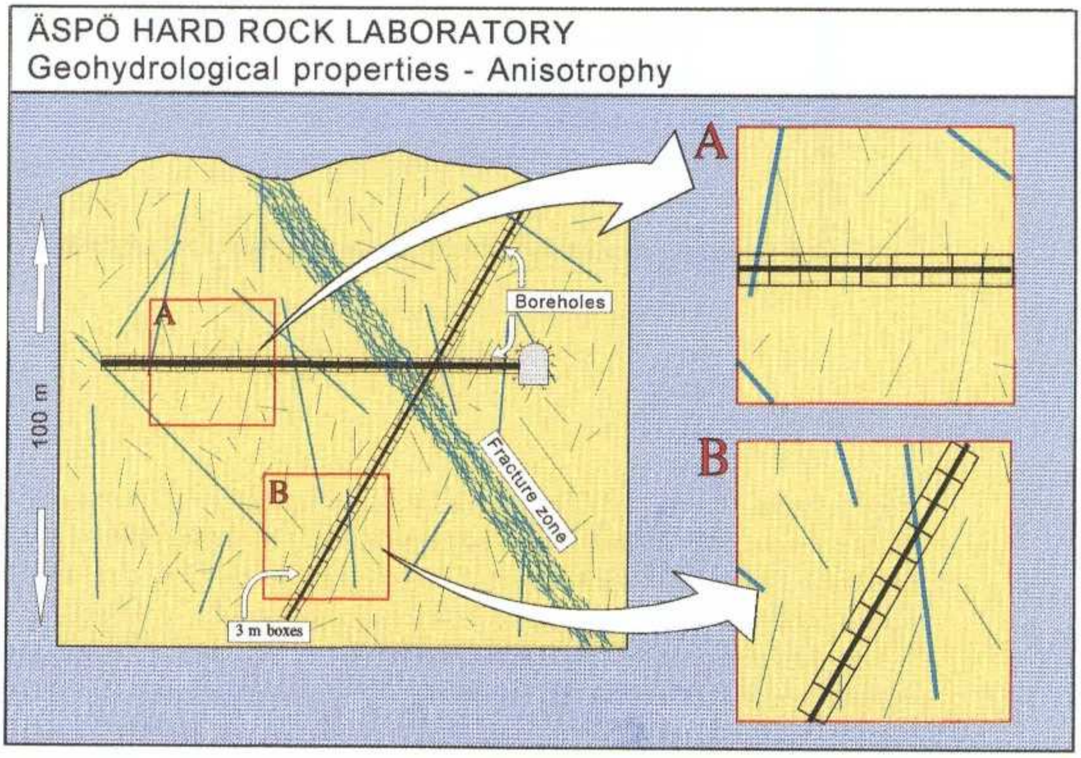


Figure 5-17. The evaluated hydraulic properties are dependent on the borehole direction if there are anisotropic conditions.

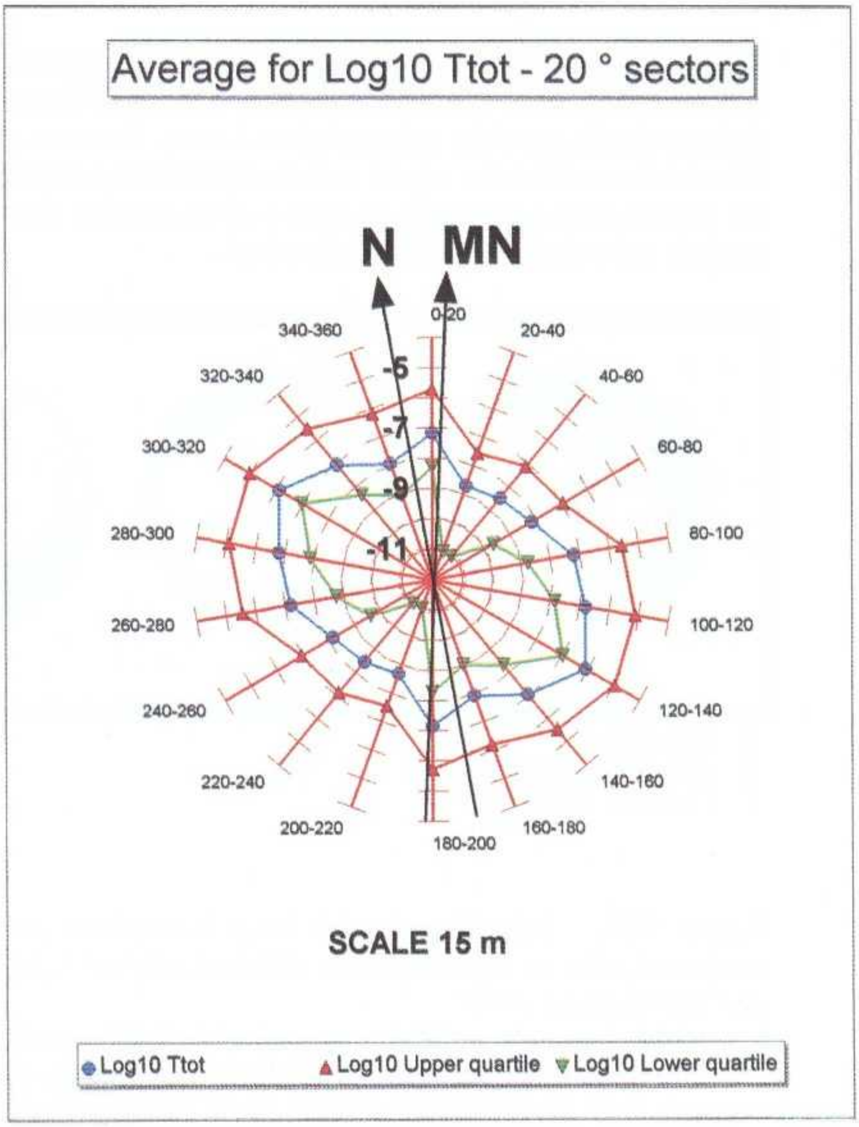
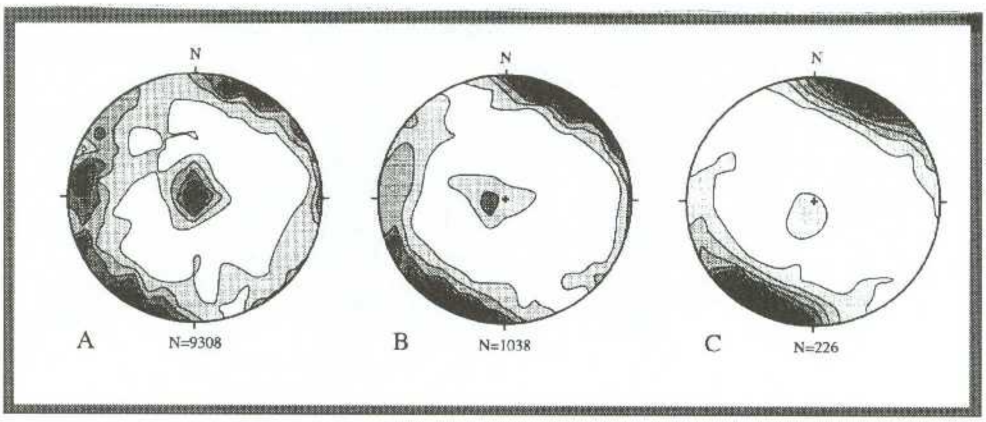


Figure 5-18. *Estimated transmissivities (T) for different directions according to the Äspö co-ordinate system in the spiral of the Äspö HRL. The direction is given as the strike of a plane perpendicular to the borehole. Data : probe holes in tunnel section 1400-3600 m. The points in the figure represents arithmetic mean, upper quartile and lower quartile of* Log_{10} *(T) for planes within a 20° sector in the horizontal plane. The points are in the middle of the sector and the directions of the sector is given for the Äspö co-ordinate system. N = North for the Äspö co-ordinate system. MN = Magnetic North. Scale 15 m = Length of test section is 15 m.*

An investigation of the structural geology of water-bearing fractures was made in the tunnel */Hermanson, 1995/*. It was found that the entire fracture system can be grouped into five main sets. The mapped water-bearing fractures and the fractures filled with grout (from the pre-grouting ahead of the tunnel face) are dominated by a subvertical fracture set striking WNW-NW. The N-S and NNW-SSW subvertical sets are also present but these subvertical sets are less pronounced compared with the entire fracture set (see *Figure 5-19*). The relevance of the orientation of the mapped water-bearing fractures can be questioned as the zone closest to the tunnel wall was damaged to some extent by the excavation, giving increased fracturing and possibly a change in the hydraulic properties. Due to this the flow paths near the tunnel wall may be different than those of the undisturbed rock mass. However, the mapped grout-filled fractures should be a good indicator of the water conducting fractures, as the grouting was performed generally 5-15 m ahead of the tunnel face where the rock mass should be fairly undisturbed.



A : All fractures
B : Waterbearing fractures
C : Fractures filled with grout

Figure 5-19. *Schmidt nets with lower hemisphere projection of Kamb contoured poles to fracture planes. Contour interval 2.0 sigma. N= sample size. /Hermanson, 1995/.*

A: *All fractures from 705 m to the end of the TBM tunnel, 3600 m. The plot shows five concentrations of fracture orientations, one sub-horizontal set, four steep sets striking N-S, NNW, WNW-NW and a comparatively less pronounced NE set.*

B: *Water-bearing fractures from the same part of the tunnel as A. The steep set striking WNW-NW is more pronounced compared with the same set in plot A. The other sets are less evident.*

C: *Fractures with grout from the same part of the tunnel as A. The plot is dominated by steep fractures striking WNW-NW. All other sets mentioned earlier are still visible, though not as pronounced as the WNW-NW set.*

A mapping campaign of major larger (intersecting the entire tunnel) water-bearing fractures in the spiral showed that all mapped fractures either had a substantial water inflow and/or grout and often gouge, brecciation or ductile precursors */Hermanson, 1995/*. They were not in any case classified as zones and their widths ranged from millimetres to centimetres. *Figure 5-20* shows the mapped fractures. The fractures shown were mainly subvertical. According to *Hermanson /1995/* the fault system trending NW and NNW generally appears as sub-planar fractures with a central water-bearing fault plane that often contains fault breccia and/or fault gouge as well as mineral assemblage.

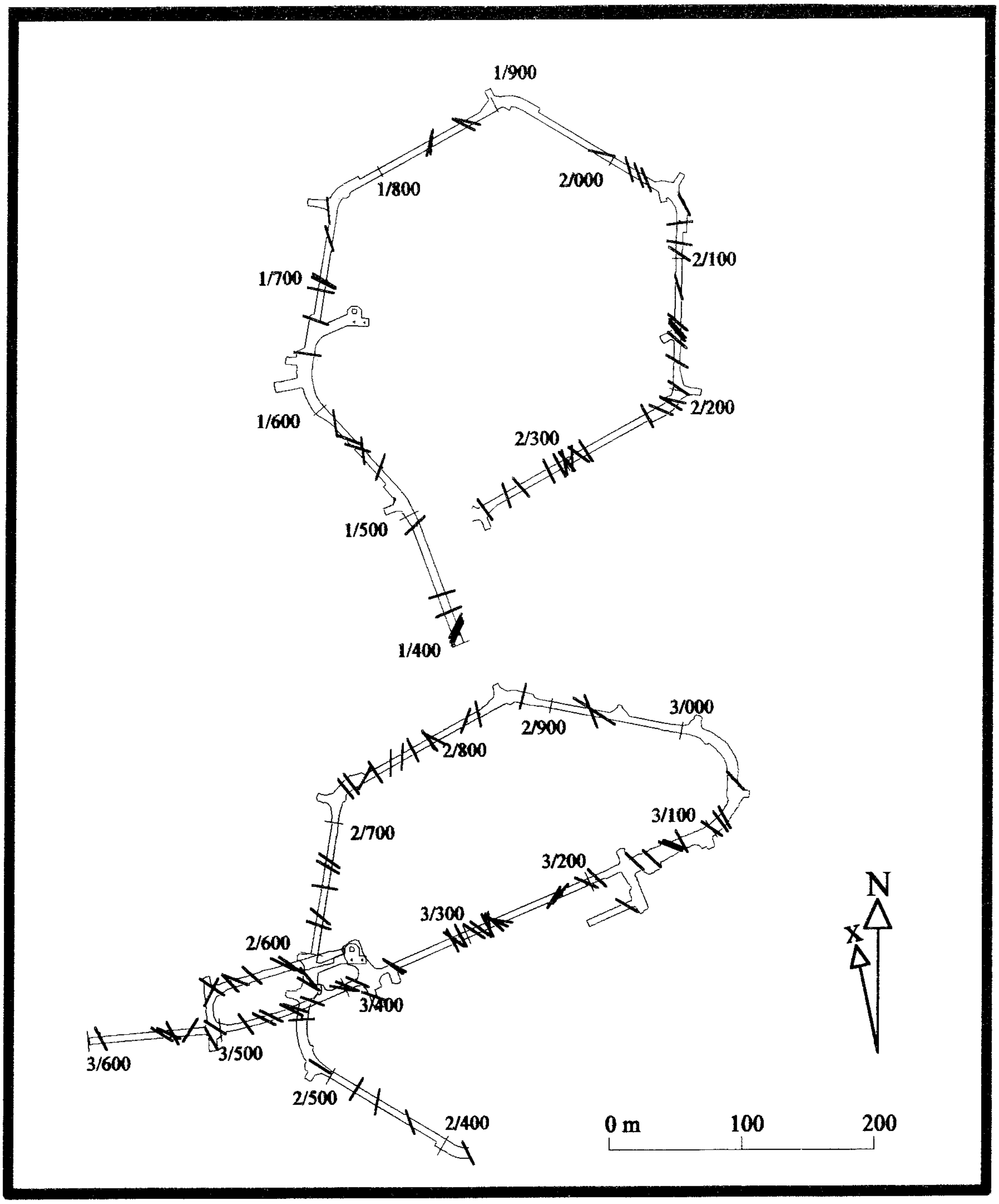


Figure 5-20. Mapped large, single, open, water-bearing fractures in the tunnel. The fractures are mainly subvertical. N = Magnetic north, x = North in the Äspö co-ordinate system.

5.4 SPATIAL ASSIGNMENT METHODS

Transmissivities (T) for the hydraulic conductor domains are assigned deterministically. T is based on transient hydraulic tests in most cases. When no hydraulic tests have been performed in a structure, T is sometimes based on geological classification combined with the evaluated transmissivities for the hydraulic conductor domains at Äspö.

The concept used for assigning hydraulic properties to the hydraulic rock mass domains is that the hydraulic conductivity within the domain can be described using a lognormal distribution, which depends on the scale of the discretisation in the flow model. No spatial correlation is assumed between the cells used in the flow model.

Hydraulic conductor domains

The assignment of the transmissivity as a constant value for each hydraulic conductor domain seems useful if solely the hydraulic potential within the model is considered. The numerical groundwater flow modelling shows that the measured hydraulic potential can be described fairly well using the hydraulic conductor domains and their transmissivities given in the descriptive hydrogeological model */Wikberg et al, 1991, Svensson 1991, 1994, 1995b, Gustafson and Ström, 1995/* (see also *Section 5.6).* A stochastically distributed transmissivity within a hydraulic conductor domain would be more realistic but has only been tested so far on the site scale */Svensson, 1994/* and on the detailed scale for a fracture */Kuylenstierna and Svensson, 1994/.* The evaluated properties indicate that the standard deviation for the Log_{10} (transmissivity) is about 0.5 to 1. The number of samples per domain is so small (see *Figure 5-13*), that it is difficult to judge if lognormal distribution (or any other distribution) of the transmissivity values for a domain is justified in general, but the more transmissive domains with sample size larger than 4 data points seem to be of approximately lognormal distribution. The sample sizes were also so small that it was not justifiable to estimate a correlation model within a domain. It is a difficult task to decide the design of tests and the number of tests needed to find estimate of the correlation models within the hydraulic conductor domains. Probably one needs many and well-controlled tests. A specific problem is for example how to evaluate the support scale (or influence radius) for an effective parameter that is evaluated.

There does not seem to be any significant change in the transmissivity with depth for the domains at Äspö */Rhén et al, 1997a/.*

Hydraulic rock mass domains

The hydraulic conductivities based on measurements has a more or less lognormal distribution (see *Figure 5-21).* The figure shows normal probability plots and a frequency plot of $\mathrm{Log}_{10}(K)$. The diagrams are based on tests at different test scales (3, 30, 100 and 'entire hole') performed in boreholes KLX01, KAS02-08. The tests at the 30 and 100 m scales were not performed systematically in all boreholes, giving some uncertainty in the interpretation that follows here. From *Figure 5-21* it can be seen that it is convenient to evaluate the mean and standard deviation for $\mathrm{Log}_{10}(K)$ and describe the population characteristics using these values as the distributions are more or less lognormal. The assumption that the population can be described by a lognormal distribution makes it easy to generate the hydraulic conductivity

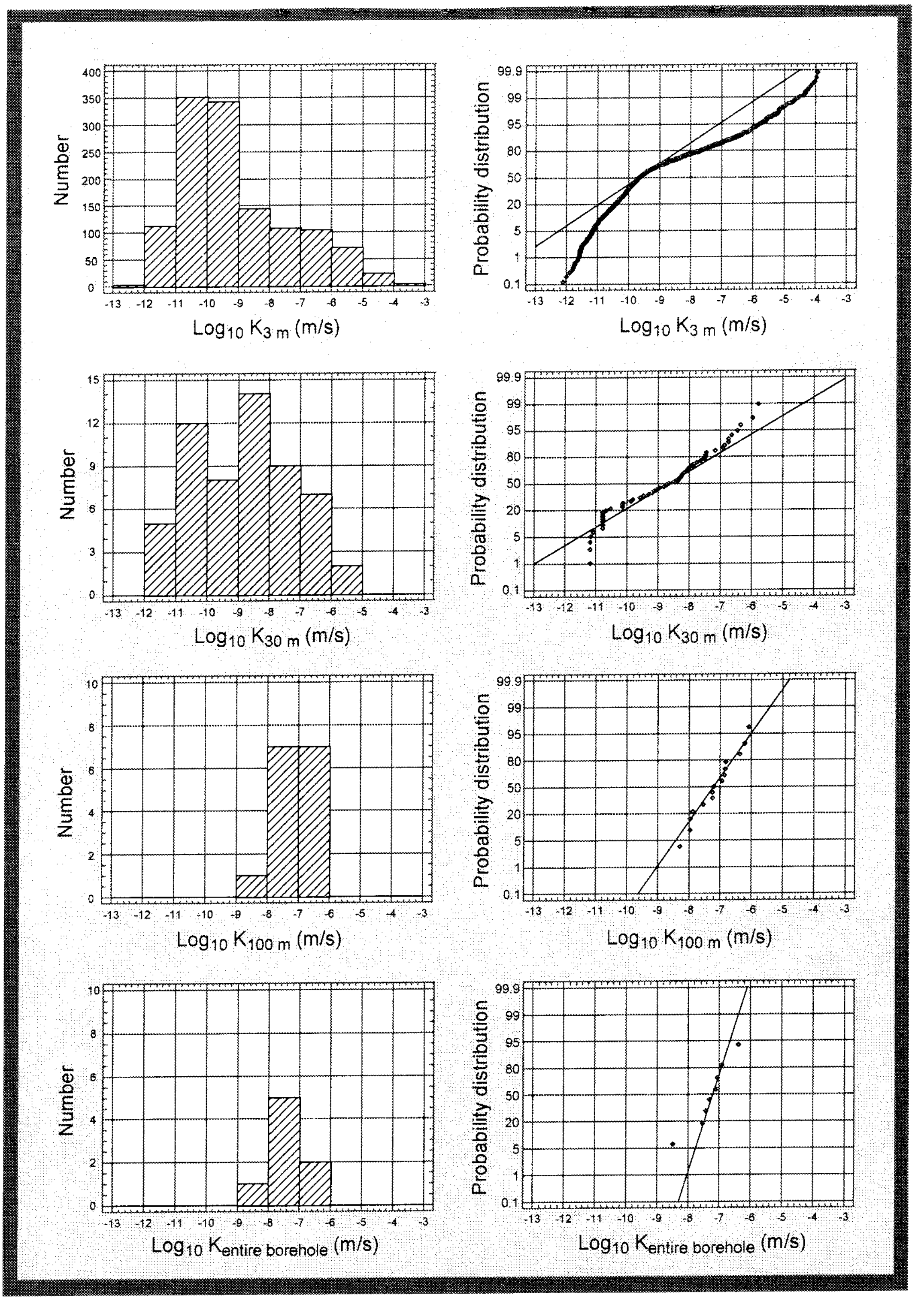


Figure 5-21. *Normal probability plots and frequency plots of Log*$_{10}$*(K), where K = effective hydraulic conductivity in m/s, for different test scales. (In the figure, for example, the 3 m test scale is shown as* K_{3m} *). Data are from the pre-investigation phase, including boreholes KLX01, KAS02-08.*

field in a stochastic continuum model - where effective values of hydraulic conductivity have to be used. However, the way of using the values in a numerical model is not obvious. The mean of $Log_{10}(K)$ is equal to the geometric mean of K, and, as can be seen in *Figure 5-21*, both the geometric mean of K and the standard deviation of $Log_{10}(K)$ change with the test scale. In the cases shown the test times also increase from about 10 minutes to 3 days. The evaluated arithmetic mean of K, geometric mean of K and standard deviation of $Log_{10}(K)$ are shown in *Figure 5-23*. It can be argued that the great change in geometric mean in *Figure 5-23* is due to the way in which the characteristic values for the distribution of the hydraulic conductivity is calculated. This is partly true since sections with higher transmissivities will always dominate the statistics increasingly with increasing test scale.

Figure 5-22 shows the results of a synthetic data set for test scales 30 m, 90 m and 'entire boreholes' (chosen as an even number of 90 m sections) calculated from the 3 m injection tests. The transmissivities were calculated for the section (30, 90 m or 'entire borehole') as the sum of the 3 m transmissivities and then divided by the section length (30, 90 m or 'entire borehole'). As 'entire borehole' was not exactly the same section as in *Figure 5-21*, two cases with synthetic data were calculated starting from the bottom or top borehole sections for the boreholes in *Figure 5-21*. Only one of these cases is shown in *Figure 5-22* as the other is almost identical. The evaluated arithmetic mean of K and geometric mean of K and standard deviation of $Log_{10}(K)$ are shown in *Figure 5-23* for the real and synthetic cases. As can be seen the geometric mean behaves in a similar way for the synthetic case and the data based on different test sections, which is not strange at all. More interesting is the arithmetic mean, which decreases with increasing test scale and test time for the real case but is constant for the synthetic data. This is interpreted as good evidence that the connectivity between the fractures is limited (see illustrations in *Figure 5-24*). True scale effects exist! *Figure 5-23* illustrates well the problem of defining an effective hydraulic conductivity as a single value for a homogeneous case or a statistical distribution appropriate for a stochastic simulation. How this problem has been handled so far and the probable reasons behind the behaviour of the statistics is discussed below.

The relations for the geometric mean and standard deviation shown on the left in *Figure 5-25* were used to scale the hydraulic conductivities used in the numerical groundwater flow models in *Model 96 /Rhén et al, 1997b/*. A similar relationship was used for *Model 90 /Wikberg et al, 1991/*. The use of a linear relationship as suggested in *Figure 5-25* can be discussed. It was used because it was not considered justified to use a more complicated relationship. The linear relationship cannot be used for test scales larger than $\log_{10}$ scale ~2.7 ≈500 m, which is the maximum length of test section used in the individual boreholes. Possibly it should not be used for scales larger than about 200 m. As can be seen in the figures there is a spread of K_a and K_g values for test scale ≈500 m indicating a standard deviation that probably should be taken into account considering scaling of values for a site and not just a borehole. However, several other functions give about the same correlation coefficients as the linear fit and the functions can be made to converge asymptotically to the

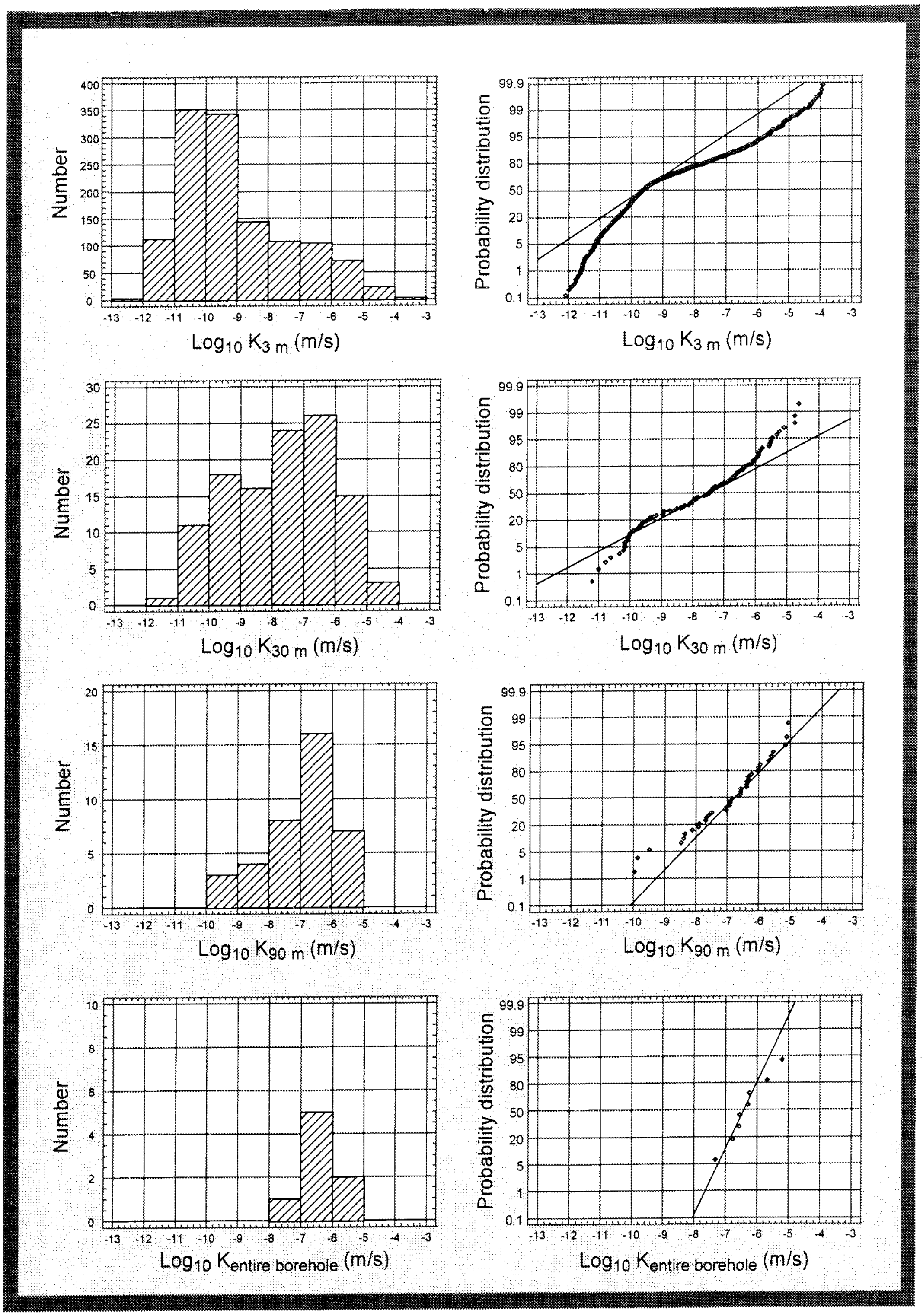


Figure 5-22. *Normal probability plots and frequency plots for* Log_{10} *(K). K = effective hydraulic conductivity in m/s. The base for the presented data is the injection tests with packer spacing 3 m in boreholes KLX01, KAS02-08. The diagrams for 30, 90 and 'entire borehole' are based on the tests on the 3 m scale by calculating the transmissivity for the section 30, 90 m 'entire hole' divided by the length 30, 90 m or 'entire hole' for more or less the same part of each borehole as was used in Figure 5-21 (see text for comments). (In the figure, for example, the 3 m test scale is shown as* K_{3m} *.)*

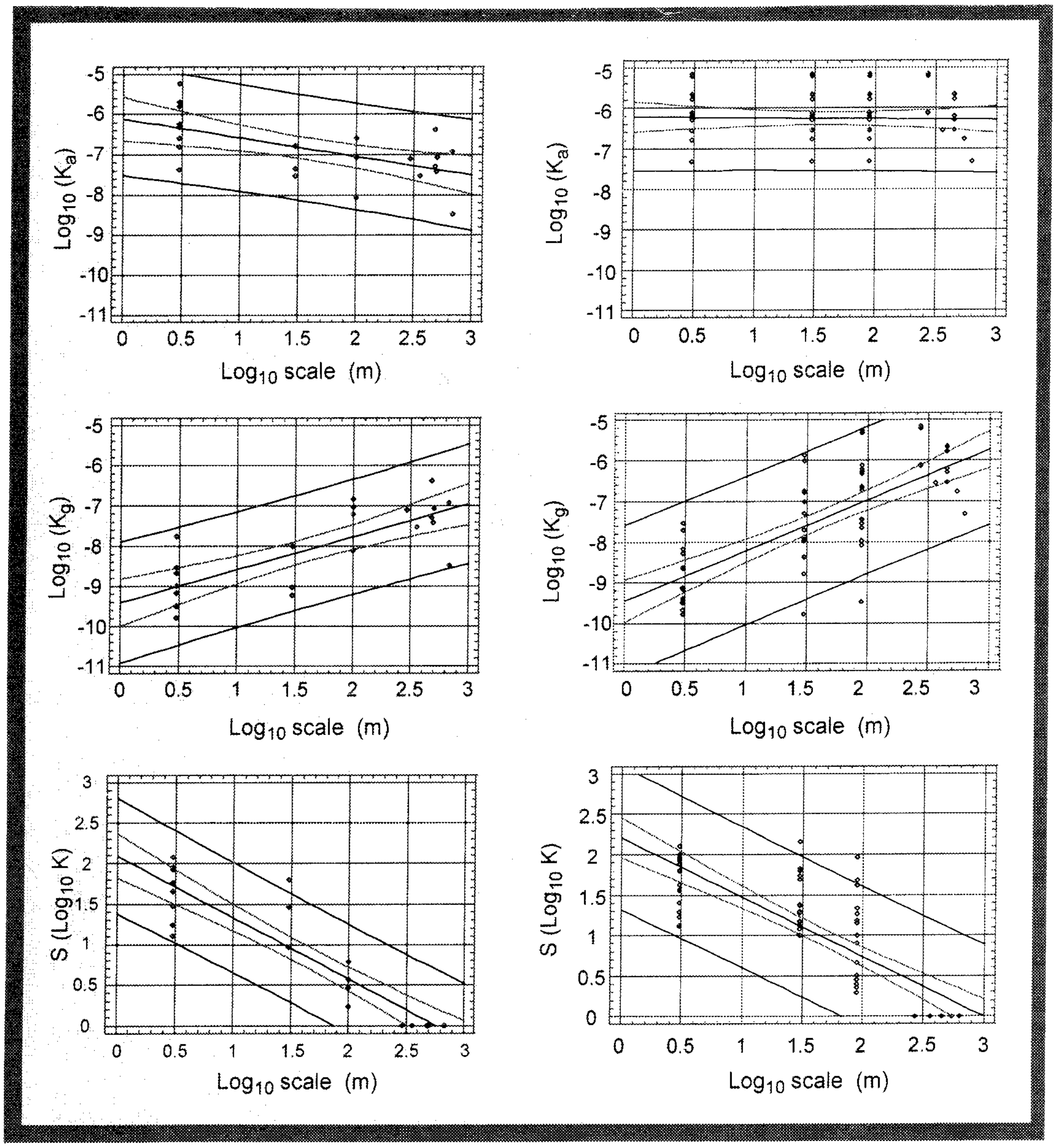


Figure 5-23. *Regression of Y versus Log_{10} (scale). Y = $Log_{10}(K_a)$, $Log_{10}(K_g)$ or s($Log_{10}(K)$). K = hydraulic conductivity, K_a = arithmetic mean of K, K_g = geometric mean of K. Scale = length of test section in the borehole. The values of K_g, and K_a for Log_{10} scale ≈2.5-3 are identical as they are the effective hydraulic conductivity for the entire borehole. Data are from the pre-investigation phase, including boreholes KLX01, KAS02-08. (Standard deviation was set to zero for the 'entire borehole' value as there is only one value for K_a and K_a.)*

Middle black line: Mean of Y.

Inner grey lines : 95 % confidence band on mean of Y.

Outer most black lines : 95 % prediction band on Y as a function of Log_{10}(scale).

Left figure: Data from the pre-investigation phase where tests were made on different test scales (see Figure 5-21).

Right figure: Synthetic data based on the 3 m injection tests (see Figure 5-22).

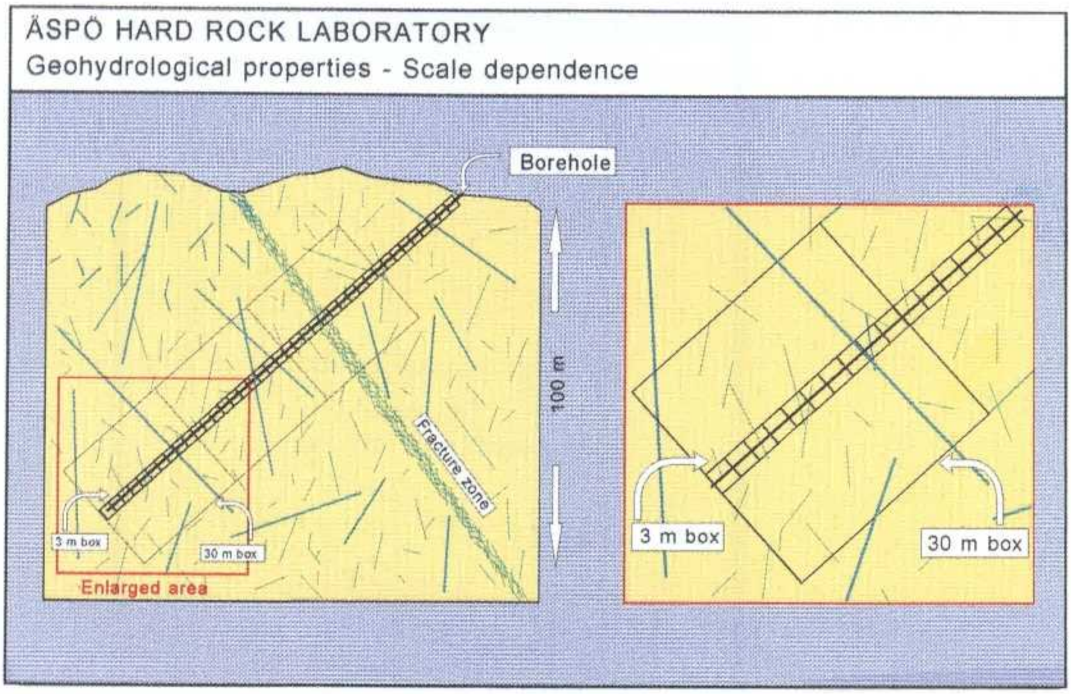


Figure 5-24. *The evaluated hydraulic properties are dependent on the test scale (length of the tested section) and test time. Larger test scales and longer test time result in fewer fractures being hydraulically active for the duration of the test. Some of the minor features intersecting the boreholes have no or poor connection with other conductive features.*

estimated values for the entire borehole. The difference will be larger correction for smaller test scale, (less than about 3 m) and smaller corrections for larger test scales (>3 m).

A few spatial correlation studies have been made: Variogram models in 1-D and 3-D, based on the injection tests from the surface with a 3 m packer spacing, indicate that the hydraulic conductivity is dominated by a random component */Rhén et al, 1997a, Niemi, 1995, La Pointe, 1994/.* In all studies all data were used, thus including both hydraulic rock mass domains and hydraulic conductor domains. The evaluated correlation ranges are around 20 to 70 m and the modellers assumed that isotropic conditions prevailed. However, the hydraulic conditions at the Äspö HRL are anisotropic and the correlation ranges may be different in different directions. The correlation range is fairly short compared with the cell size in the numerical model and, what is more important, the nuggets in the variogram models are large (generally about 60% of the total variance). The assumption of no correlation between the 20 • 20 • 20 m cells on the site scale numerical models seems justified, based on the correlation models mentioned above.

However, there is most likely too little correlation in the stochastic model without any correlation structure for features with higher transmissivities when cell sizes in the numerical model are tens of metres or less with the modelling approach used so far. The radius of influence for a specific test depends on the

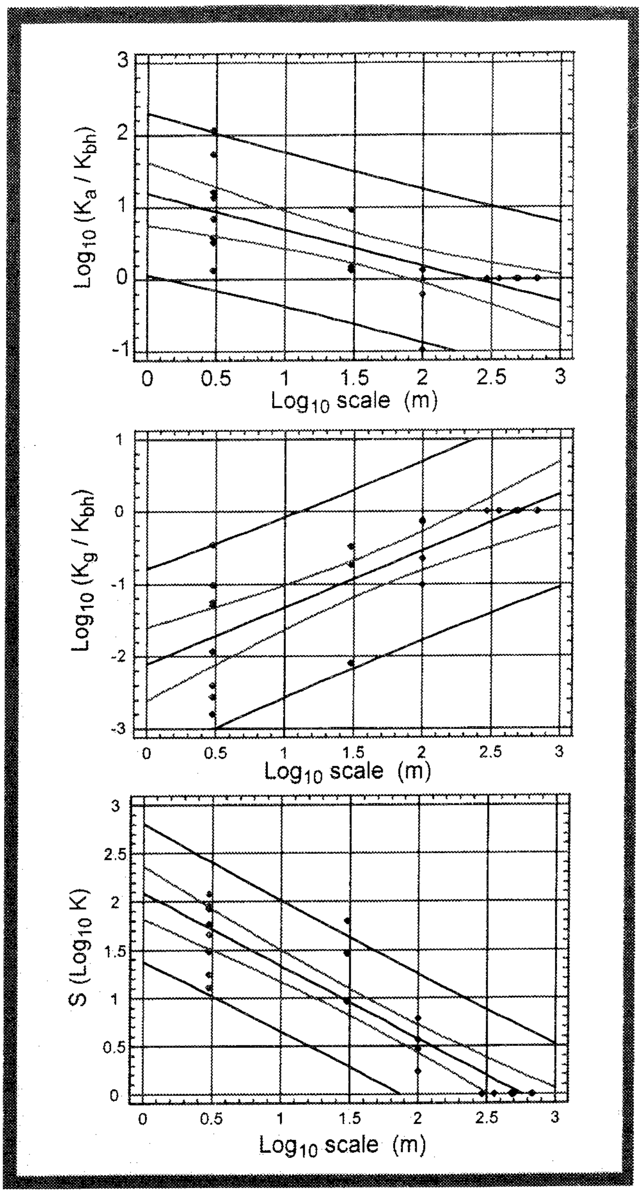


Figure 5-25. *Regression of Y versus* Log_{10} *(scale).* $Y = Log_{10}(K_a/K_{bh})$, $Log_{10}(K_g/K_{bh})$ *or* $s(Log_{10}(K))$. *K = hydraulic conductivity,* K_a *= arithmetic mean K,* K_g *= geometric mean K.* K_{bh} *= mean K when entire borehole was tested, corrected according to test sections outside the range for other test scales. Scale = test section length in the borehole. The values of* K_g *and* K_a *for* Log_{10} *scale ≈2.5-3 are identical as they are the effective hydraulic conductivity for the entire borehole. The linear relation should not be used for test scales larger than* log_{10} *scale ~2.3 ≈200 m. Data are from the pre-investigation phase, including boreholes KLX01, KAS02-08. (Standard deviation was set to zero for the 'entire borehole' value as there is only one value for* K_a *and* K_a*).*

Middle black line:	*Mean of Y.*
Inner grey lines :	*95 % confidence band on mean of Y.*
Outer most black lines :	*95 % prediction band on Y as a function of* Log_{10}*(scale).*

hydraulic properties around the borehole. So far, the radius of influence has just been estimated roughly using the test section length as an indication of mean influence radius. Using the suggested relationships between hydraulic conductivity and specific storativity shown in *Rhén et al /1997b/* the arithmetic mean influence radius is about 6, 22, 17 and 62 m for test scales 3, 15, 30 and 100 m respectively, using the simple approach of radial flow (see *Figure 5-26).* (Total test time was used if no upper time for the evaluation period was given.) The values above and in *Figure 5-26* should be seen as indications of influence region and not absolute values. The radius of influence linked to the evaluated hydraulic property can possibly be evaluated and incorporated into the model description, thus improving the base for a spatial correlation model.

In order to see if it was possible to estimate effective values of the hydraulic conductivity of a rock block measuring 50 m simulations using a Discrete Fracture Network (DFN) model were made */Axelsson et al, 1990, La Point et al, 1995/.* The first attempt was not successful as it turned out that the results depended very much on the boundary conditions. The simulations performed in *La Point et al /1995/* suggest that the conductive network was sparsely connected and that the block permeability decreases when the block size exceed the scale of well-connected fracture networks. The results showed that the block permeability was sensitive to the mean fracture size and fracture intensity, not surprisingly. They also noted that anisotropic conditions may exist with the permeability (k) in the north-south direction, followed by the k in the vertical direction and with the k in the east-west direction that was evaluated to be the least. The results also showed a need for improved data collection and better methodology for using the well test data in the numerical models. A good representation in 3-D of mapped fracture intersections in boreholes and fracture traces on rock surfaces is needed to improve the description of the orientation- and size distributions of the fractures, and also fracture intensity. A difficulty in the mapping and testing in boreholes is to distinguish water-conducting fractures and non-water-conducting fractures, which also affects the modelling.

The reasons for the scale dependency seen in the evaluated statistical properties are:

- The hydraulically active fractures are sparsely distributed and not very well interconnected hydraulically.

- Longer test time result in fewer fractures being hydraulically active. Some of the minor features intersecting the boreholes have no or poor connection with other conductive features and with increasing test time the flow will decrease in these features. The larger and more transmissive features will control the flow towards the borehole.

- Part of the scale dependency observed, is due to the way in which the statistical properties are calculated. Features with large transmissivities will dominate the statistics for larger test sections.

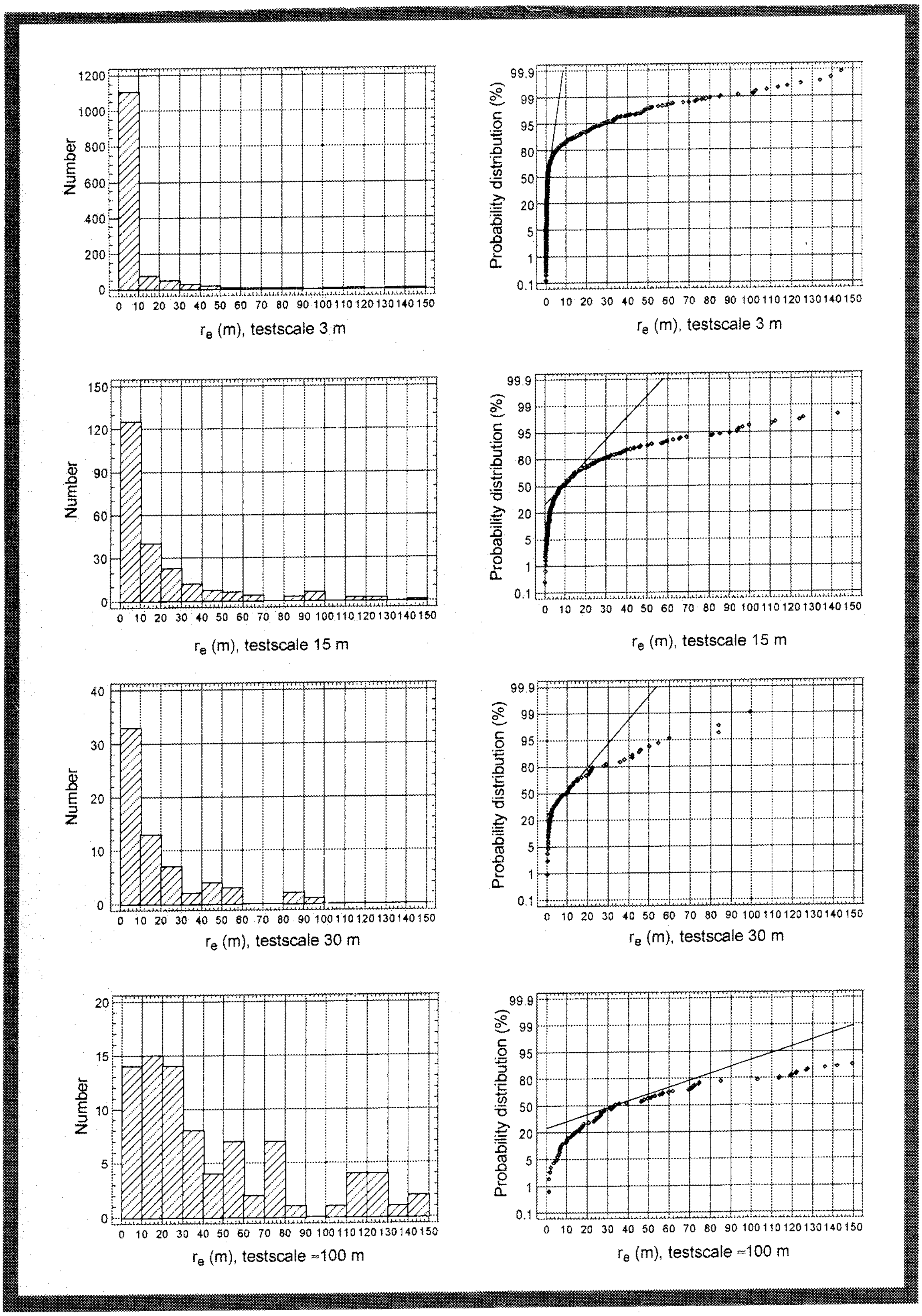


Figure 5-26. *Indication of radius of influence assuming a power law relationship between specific storativity and hydraulic conductivity according to Rhén et al /1997b/ and radial flow. Data from the pre-investigation and construction phase at Äspö HRL. Total test time was used if no upper time for the evaluation period was given.*

5.5 MONITORING OF WATER PRESSURES, PRECIPITATION, ETC.

During both the pre-investigation and construction phases, the air temperature, precipitation and sea level were measured for neighbouring areas. The potential evapotranspiration and run-off for some nearby areas were also estimated */Rhén et al, 1997b/.* These measurements form the base for defining the upper boundary conditions for groundwater flow models. A main effort during both investigation phases was the monitoring of the water pressures in the rock mass. These measurements form a base for defining the vertical boundary conditions in groundwater models. By means of the relatively intense measurement of the water pressures it was possible to gain a better understanding of the influence of the barometric pressure, sea level and tidal effects on the pressures and also the groundwater recharge due to the precipitation.

The piezometric levels of the groundwater in the Äspö, Ävrö and Laxemar, areas were measured in a large number of boreholes drilled from ground level (see *Figure 5-27* and *5-28).* The percussion boreholes, generally 100-200 m deep, contained 1-3 measurement sections. The coreholes, which are up to 1000 m deep, had up to 6 measurement sections. Some of the boreholes drilled from the tunnel were also equipped with packers and connected to the monitoring system in the tunnel. The monitoring system is described in more detail in *Almén and Zellman /1991/* and *Almén and Johansson /1992/.*

The monitoring of the water pressures in the rock mass was used for:

- interpreting interference tests,
- interpreting hydraulic responses during the excavation of the Äspö tunnel,
- interpreting hydraulic responses during drilling from the tunnel,
- measuring the natural water pressures (undisturbed by the tunnel) and
- measuring the drawdown during excavation.

The measured data are very important for the numerical groundwater simulations. The data were used for calibrating the groundwater flow models and to test how well the models reproduce the measured pressures. The boundary conditions used in the numerical groundwater flow simulations are presented in *Section 5.6.*

The absolute pressure along parts of the coreholes was also estimated from the transient injection tests with a packer spacing of 3 m. These estimates were considered uncertain as the pressure-transducers used and calibration procedures were not aimed at getting a good resolution of the absolute pressures. The pressure distribution along the boreholes is useful to know so the flow directions in the borehole before packer installation can be estimated and used for interpretation of the water chemical sampling, and also the temperature and resistivity logging in open boreholes. As mentioned above, it is also important to have reliable measurements of the natural (undisturbed) pressures for the assessments of the boundary and initial conditions in the numerical models. Hydraulic tests and monitoring can provide these data.

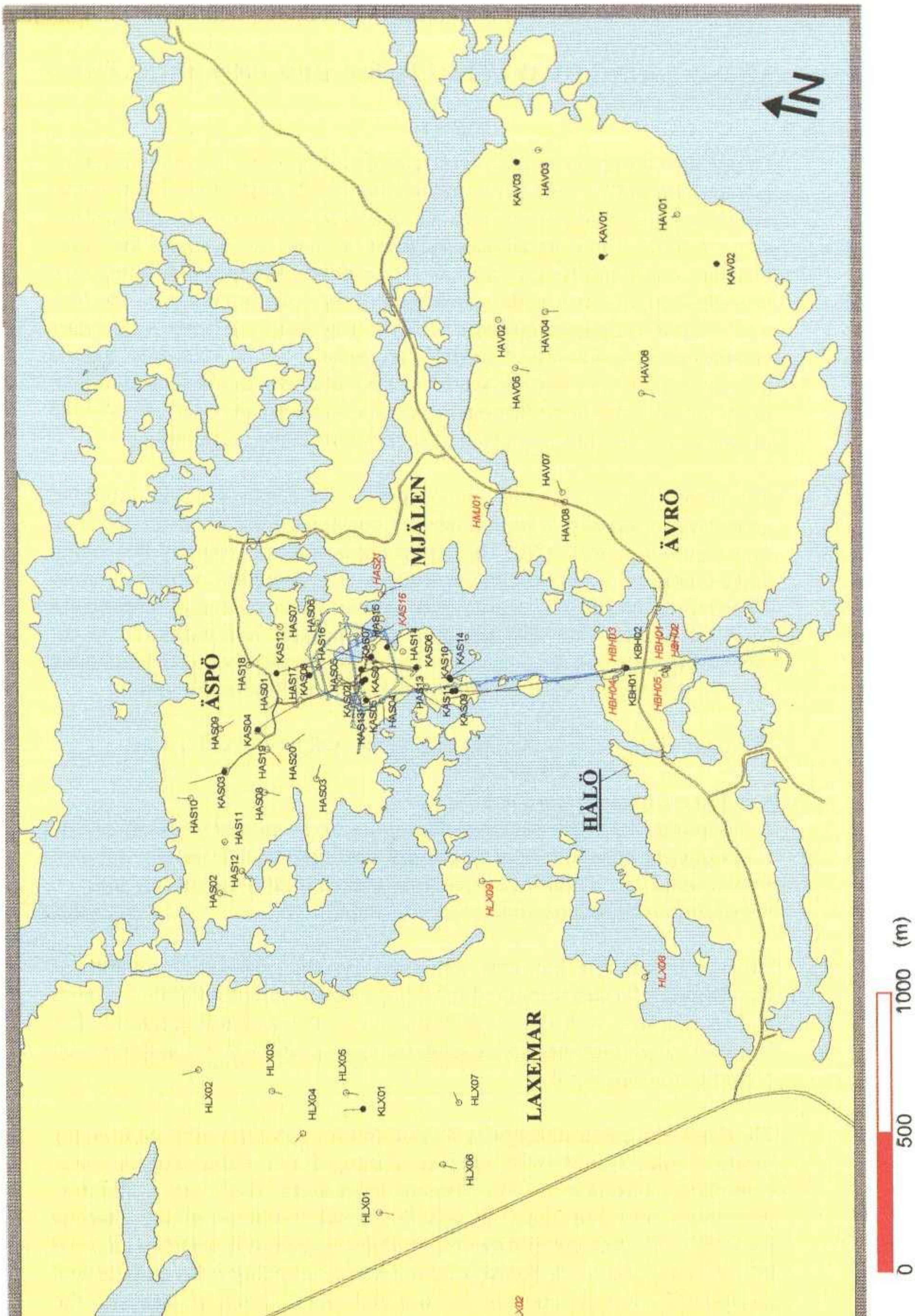


Figure 5-27. Plan of the boreholes (black label) included in the predictions of the piezometric levels reported in Rhén et al /1991 /. Boreholes with a red label were drilled during the construction of the Äspö HRL. Filled circles: Cored boreholes. Un-filled circles: Percussion boreholes.

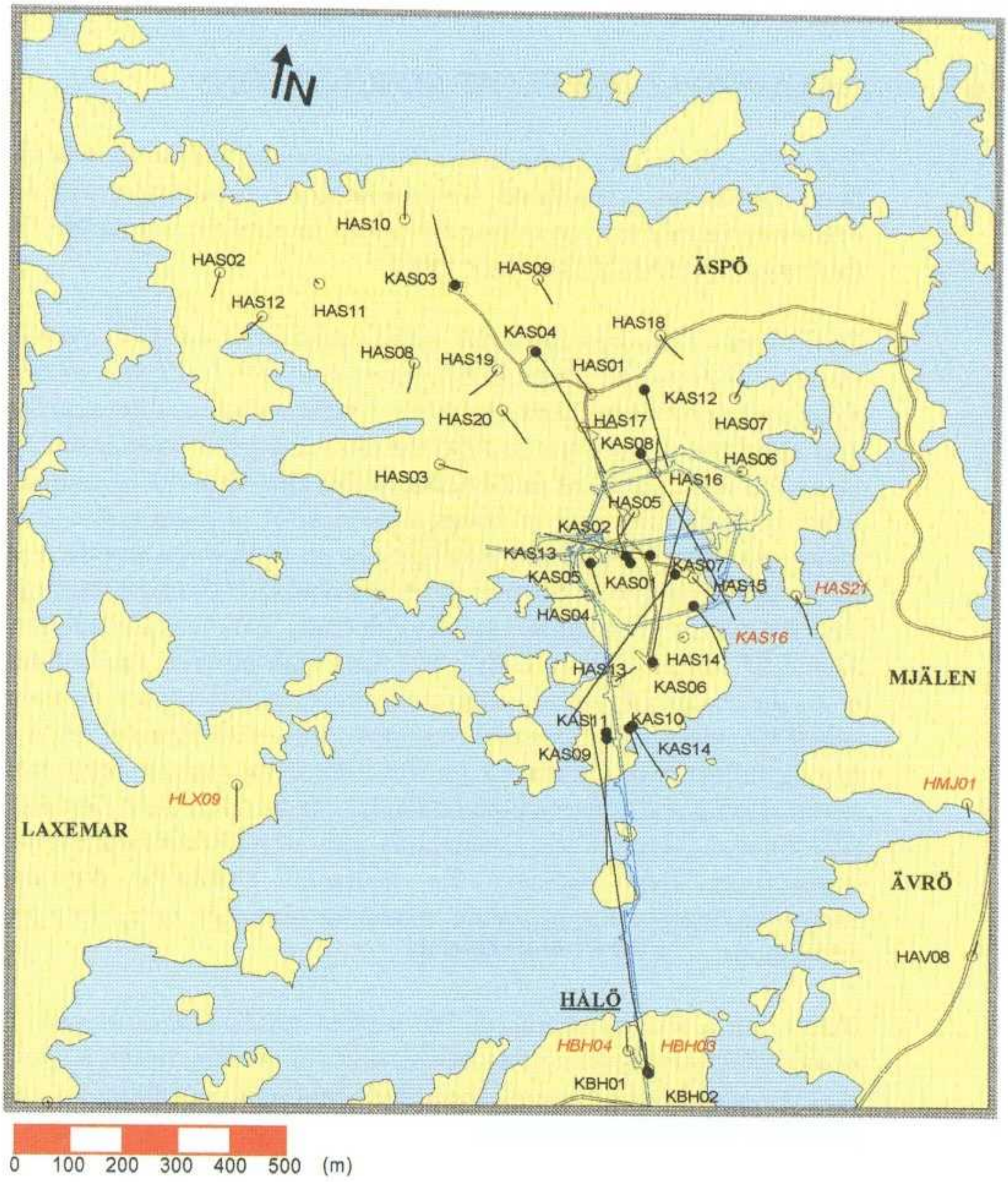


Figure 5-28. *Plan of the boreholes (black label) included in the predictions of the piezometric levels reported in Rhén et al /1991/. Boreholes with a red label were drilled during the construction of the Äspö HRL. Filled circles: Cored boreholes. Un-filled circles: Percussion boreholes.*

5.6 GROUNDWATER FLOW SIMULATIONS

The data in the model presented in *Wikberg et al /1991/* were used to make a three-dimensional groundwater flow model that was calibrated with a number of the interference tests as well as the natural level of the water table. The code used was PHOENICS */Spalding, 1981/.*

Predictions of the drawdown due to the construction of the Äspö HRL were made in 1990 and presented in *Gustafson et al /1991/, Rhén et al /1991/* and *Svensson /1991/* (here called *Model 90*). The boundary condition in the tunnel was atmospheric pressure. In 1995 the drawdown was once again calculated using the same model as in 1990 but in that case with the measured flow of water into the tunnel up to tunnel section 2874 m (here called *Recalc 90*) */Svensson, 1995b/*. Another modelling case in 1995 was a modified model of the hydraulic conductor domains (here called *Model 95*) and a third modelling case was with one hydraulic conductor domain (EW-5) excluded (here called *Model 95 without EW-5*). Only a few tests with different realizations of the hydraulic conductivity field within the hydraulic conductor domain, sometimes called Monte Carlo simulations, were performed with *Model 90.* It was found that the influence on the drawdown was limited and thus the predictions were based on one realization of the hydraulic conductivity field. *Recalc 90* was performed as Monte Carlo simulations with 10 realizations of the hydraulic conductivity field between the hydraulic conductor domains. The transmissivities of the hydraulic conductor domains were the same in all realisations.

Below are a few comments on the way in which *Model 96* was used for numerical groundwater simulations in order to give the reader a brief insight into the model development. The results from that modelling are, however, presented in *Rhén et al /1997b/.*

Process

The numerical model is based on the:

- Continuity equation (mass balance equation).
- Equation of motion (Darcy's law, including density-driven flow).
- Equation of state (Salinity-density relationships).

The models up to 1995 were single-phase models assuming saturated condition up to the surface. The groundwater flow simulations based on Model 96, a simplified approach to model the unsaturated conditions, were used (see *'Boundary conditions'* below).

Material properties and spatial assignment methods

For all Äspö HRL site models up to 1995 the following spatial assignment methods were used:

- The hydraulic conductivities of a hydraulic rock mass domain were given as a stochastic distribution for the domain. The distribution of K was assumed to be lognormal with characteristic values K_g (geometric mean) and s_{LOG10K} (standard deviation of $Log_{10}(K)$). K_g and s_{LOG10K} were scaled according to the cell size in the numerical model (see *Wikberg et al/1991/* for the scale relationship). No spatial correlation was assumed between the cells in the numerical model.

- The transmissivity of a hydraulic conductor domain was given as a constant value for the domain. In the numerical model the cell-wall conductivities were modified based on the intersection length of the hydraulic conductor domain on each cell-wall and the transmissivity (see *Svensson /1991/).*

The same spatial assignment methods as above are suggested for *Model 96* in *Rhén et al /1997b/* except for the scaling K_g and s_{LOG10K}, which have been updated. *Figure 5-5* and *Table 5-2* summarize suggested material properties and spatial distribution of domains.

Boundary conditions

The boundary conditions used in the numerical models up to 1995 on the site scale were:

Upper boundary:
Fixed infiltration rate on Äspö = 3 mm/year (based on calibration using the undisturbed water table), constant pressure head at sea and peat areas.

Lower boundary:
No flow.

Side boundary:
Prescribed pressure (hydrostatic with an assumed salinity distribution).
Salinity: linear increase with depth at vertical boundaries and water flowing into the model is given the salinity value corresponding to the depth at which it flows in (see *Chapter 7* - transport of solutes - for details).

Internal boundaries:
Tunnel: skin factor (local hydraulic resistance) for rock around the tunnel and prescribed pressure at tunnel wall (atmospheric, *Model 90*) **or** no skin factor for the rock around the tunnel but instead prescribed flow rate into the tunnel (*Recalc 90, Model 95* and *Model 96 without EW-5*).

The skin factor in *Model 90* was based on the following: At the outset of the project it was decided that a more or less tight tunnel was not needed and due to hydrochemical reasons the grouting should be limited and controlled. From the hydrogeological point of view it was also of interest to obtain sufficiently large inflows to get clear responses in the observation boreholes around the excavated tunnel. At the outset of the planning for the groundwater flow simulations it was decided to take into account the working environment and probable grouting in a realistic way. Accordingly, the flow into the tunnel from the deterministically defined water-bearing zones was limited to a maximum of approximately 3 l/s. Fracture zones which ungrouted would give higher flow rates than this were expected to be grouted. In the numerical model each zone intersecting the tunnel was given, if necessary, a hydraulic resistance, here called a 'skin factor', in order to maximize the flow rate to approximately 3 l/s. The skin factor of the rock between the zones was assumed to be 0 or 10. These two different values were used to test how the skin factor would affect the flow rate into the tunnel and the pressure outside the tunnel. The increase in the hydraulic resistance around the tunnel (skin factor = 10) could be due to grouting or due to changes in the hydraulic properties within the EDZ (Excavation Disturbed Zone).

In *Model 96*, as implemented in the numerical model, the groundwater recharge is dependent on the level of the water table. Drawdown increases the local groundwater recharge. The upper boundary in *Model 96* is modelled in the following way: P-E, Precipitation minus Evaporation, is set to 200 mm/year in the regional model, which is relevant for the Äspö area. Capillary forces are not considered, which means that pressure in the unsaturated zone will be equal to the atmospheric pressure, here set to zero. It then follows that the vertical conductivity, K_z, is equal to P-E close to the ground surface. This can be understood from the balance of forces:

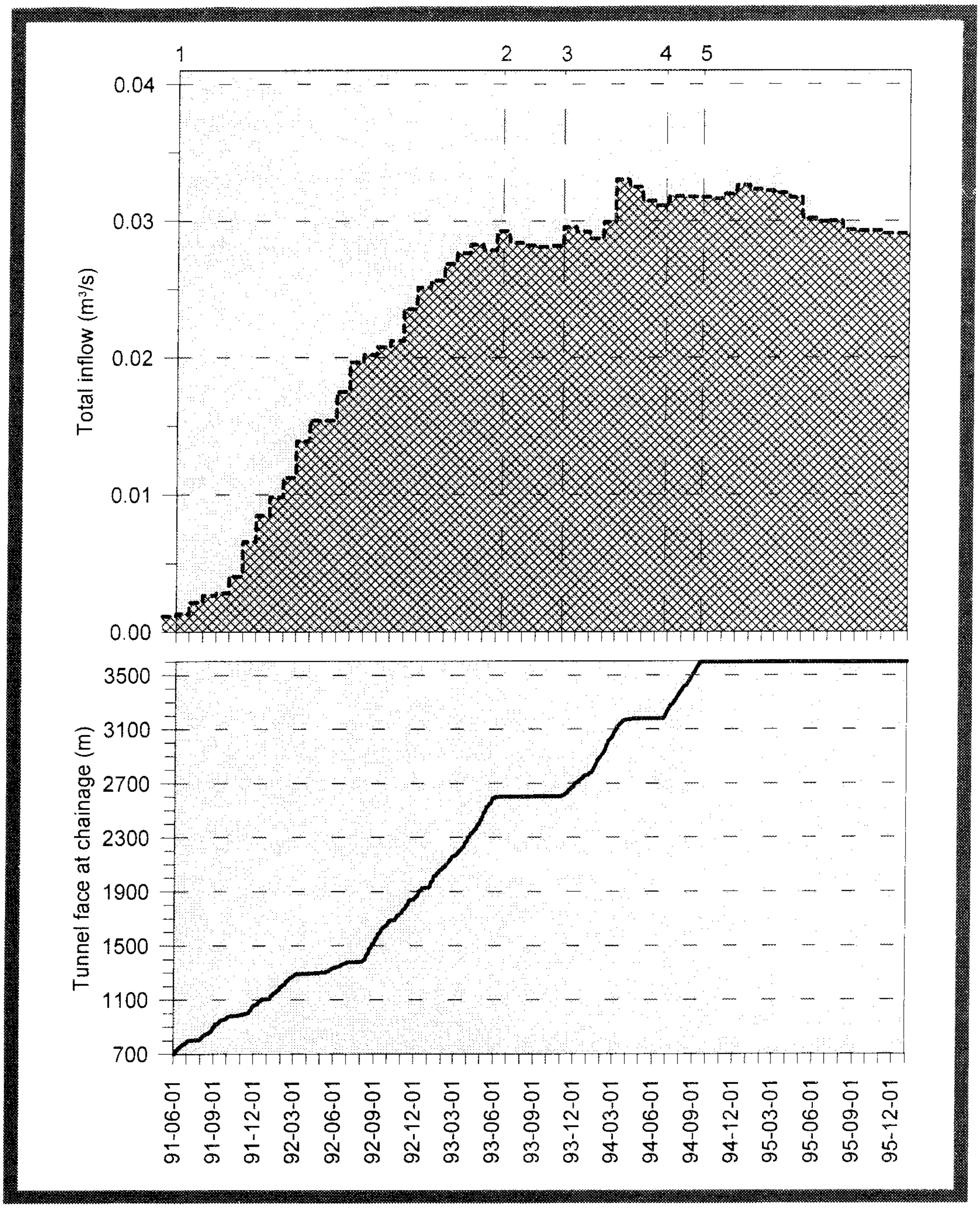
$$0 = -\frac{\delta p}{\delta z} - \frac{\rho g}{K_z} w \varphi - \varrho g,$$

where w is the vertical Darcy velocity, ϱ density and g the gravitational constant. φ is estimated by iteration in order to achieve $p = 0$ in the unsaturated zone */Svensson, 1995a/*. The resistance factor φ also reduces the horizontal hydraulic conductivities. For the unsaturated zone close to the ground $p = 0$ and $w = -(P - E)$ and hence $K_z = P - E$.

The other site scale boundary conditions for *Model 96* are taken from a larger, regional model.

Measured and predicted values - Cumulative flow into tunnel

The total net flow into the tunnel is shown in *Figure 5-29*. The prediction and outcome of the flow into tunnel section 700 - 2875 m are presented in *Figure 5-30* and *Table 5-3*. As can be seen the outcome is 84 - 93% of the prediction.



1 Passage of tunnelsection 700 m
2 Stop of excavation at 2600 m
3 Start of excavation at 2600 m
4 Start of TBM drilling
5 End of TBM drilling

Figure 5-29. *Flow into tunnel section 0 - 3600 m. The monthly inflow into the tunnel is the sum of the estimated monthly mean inflows measured at each weir /Rhén et al, 1997a/.*

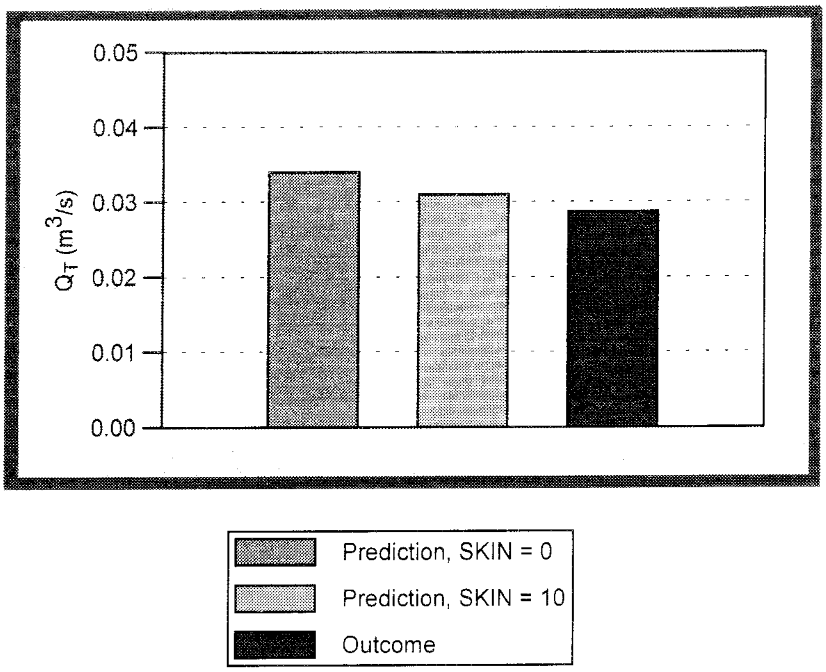


Figure 5-30. *Water flow into tunnel section 700 - 2875 m, when the tunnel face was at 2875 m. Predictions were for section 700 - 2790 m, which approximately corresponds to actual tunnel section 700-2875 m / Rhén et al, 1997a/. Predictions shown were based on Model 90.*

The decrease in flow rate during the spring of 1995 shown in *Figure 5-29* is probably due to the permanent reinforcement of the tunnels performed from January to late May 1995.

The net inflow of water in the ventilation air was approximately 0 - 0.035 · 10^{-3} m^3/s in May to August and the net outflow of water in the ventilation air was approximately 0 -0.06 · 10^{-3} m^3/s from September to April, which are small flow rates compared with the flow rates at the weirs.

Table 5-3. Water flow into tunnel section 700 - 2875 m, when the tunnel face was at 2875 m. Predictions shown were based on *Model 90.* (Skin factor = SK) */Rhén et al, 1997a/.*

Tunnel section (m)	**Outcome** (m^3/s) · 10^{-3}	**Prediction** **SK = 0** (m^3/s) · 10^{-3}	 **SK = 10** (m^3/s) · 10^{-3}	**Depth for sample** (m)
700-1475	20.2*	15	14	100-200
700 - 2265	27.6**	27.5	24.5	100-300
700-2875	28.7	34***	31***	100-400

* August 1992

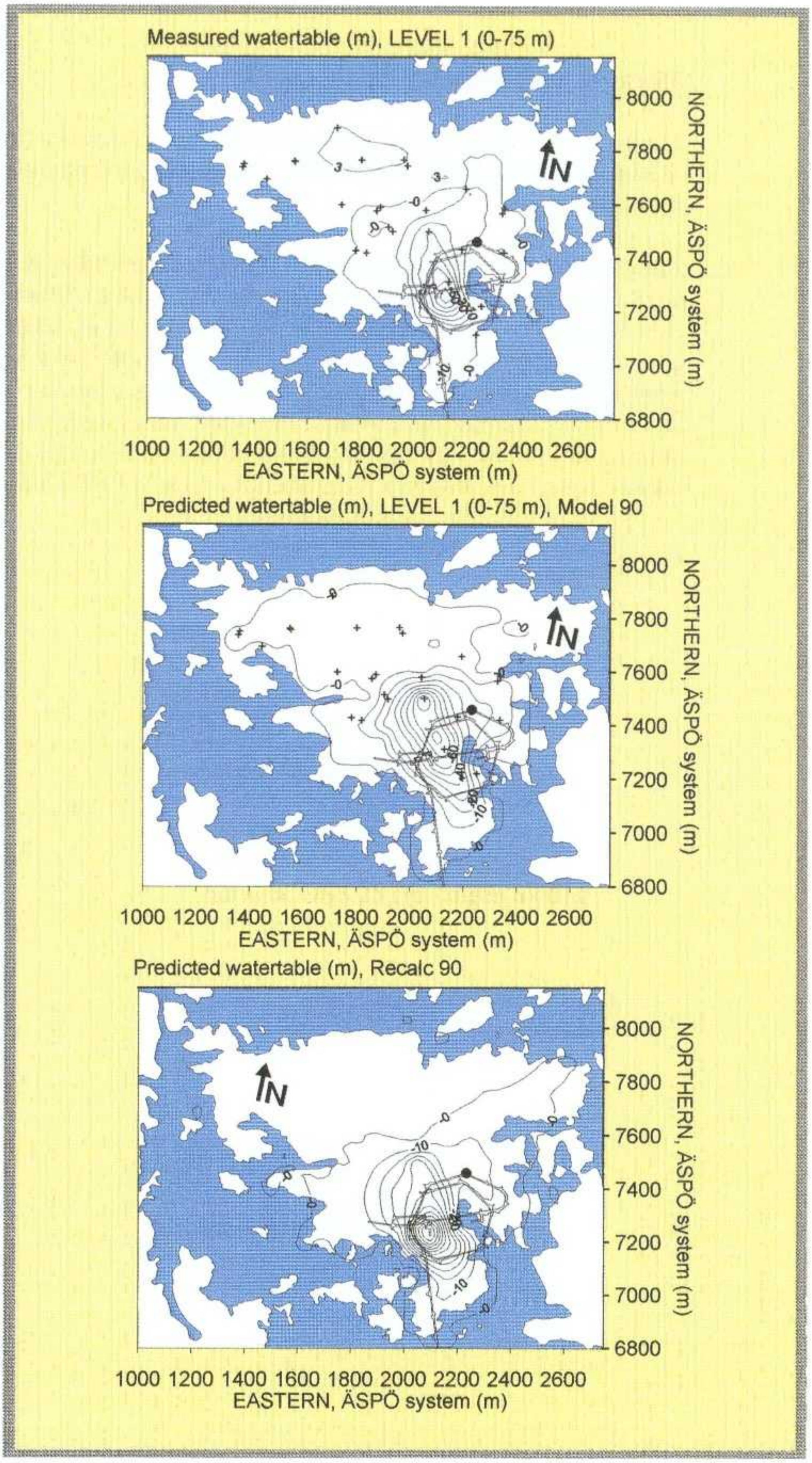
** March 1993

*** Tunnel section 700 - 2790 m according to predictions, which corresponds approximately to the actual tunnel section 700-2875 m.

Measured and predicted values - water table

Figure 5-31 shows the measured water table and the water tables based on *Model 90* and *Recalc 90*. Details of the simulations are contained in *Rhén et al /1997a/.*

The drawdown predictions made in 1990 during construction of the Äspö HRL were approximately the same as the measured drawdowns. When the measured flow into the tunnel was available the drawdown was re-calculated with the measured inflow rates but otherwise using the model 1990, the fit became somewhat less good compared with the predictions made but still the drawdowns where approximately as those measured. When the hydraulic conductor domain close to the shaft, NNW-7, was added to the model the drawdowns became better compared with the predictions made in 1990 */Rhén et al, 1997a/.*



Measured watertable (m), LEVEL 1 (0-75 m)

Predicted watertable (m), LEVEL 1 (0-75 m), Model 90

Predicted watertable (m), Recalc 90

Figure 5-31*. Water table with the tunnel face at chainage 2875 m.*

Top: Outcome. Middle: Prediction made in 1990 (Model 90).

Bottom: Prediction made in 1995 (Recalc 90). '+' shows the position of the borehole sections for the measured water level and the black dot the tunnel face position for the shown drawdown.

Summary of predictions and outcome

For comparison between different predictions the mean error and accuracy have been estimated as below. The results are shown in *Table 5-4*. The mean error and accuracy are less for *Model 95* than for *Recalc 90*. The model was also improved, in terms of decreasing lower values for dh, dh(abs) and Dh, to some extent when the subhorizontal conductor domain EW-5 was excluded.

MEAN ERROR

$$dh = \frac{\sum_{i=1}^{n} (h_i^m - h_i^c)}{n} \qquad \text{(m)}$$

$$dh(abs) = \frac{\sum_{i=1}^{n} \left| h_i^m - h_i^c \right|}{n} \qquad \text{(m)}$$

ACCURACY

$$Dh = \sqrt{\frac{\sum_{i=1}^{n} (h_i^m - h_i^c - dh)^2}{n - 1}} \qquad \text{(m)}$$

n:	Number of points with measured data, used to compare with calculated points.
h:	Piezometric level (fresh-water head) in metres above sea level (masl).
index m:	Measured value.
index c:	Calculated value.

Table 5-4. Mean error and accuracy of predictions. SK= skin factor for the tunnel.

Tunnel face position (m)	Model. year	Model	dh SK=0 (m)	dh SK=10 (m)	abs(dh) SK=0 (m)	abs(dh) SK=10 (m)	Dh SK=0 (m)	Dh SK=10 (m)
1475	1990	Model 90	0.34	-0.89	3.44	2.73	10.24	4.85
2265	1990	Model 90	6.62	-0.78	13.45	10.64	20.48	16.73
2875	1990	Model 90	12.87	5.48	16.84	10.93	22.21	14.22
2875	1995	Recalc90[1]	19.93		26.13		120.41	
2875	1995	Model95[2]-	9.03		11.02		11.23	
2875	1995	Model95[3]-	8.04		9.78		10.25	

[1] Measured flow rates into the tunnel used.

[2] Measured flow rates into the tunnel and up-dated model of the hydraulic conductor domains used.

[3] Measured flow rates into the tunnel and up-dated model of the hydraulic conductor domains used. Hydraulic conductor domain EW-5 excluded.

Conclusions

Cumulative flow into tunnel

The prediction of the total flow into the tunnel was successful, but it should also be said that the flow rate into a tunnel is difficult to predict as the amount and effect of the grouting is not known beforehand. The flow rate is more or less governed by the effect of the grouting as grouting is only performed when the tunnel intersects conductive parts of the rock mass.

It can also be added that the total flow into the tunnel after the excavation was somewhat less than the total pumping capacity of the drainage system. As a drainage system may be expensive and difficult to change it is of course interesting to make reasonably reliable predictions of the flow rate before construction is started.

From the groundwater flow modelling view point it is also important to obtain reliable measurements in time and space of the flow rates if more detailed simulations are to be made to test or calibrate the hydrogeological model. Dams should be constructed upstream and downstream of a hydraulic conductor domain, where high inflow rates are expected. One problem at the Äspö HRL was the delay in the construction of the dams and other facilities for measuring flow rates from the dams. For practical reasons it was found difficult to construct a dam closer than about 150 m from the tunnel face, if it were not to interfere too much with the excavation work. However, a number of dams were constructed far away from the tunnel face, which of course made estimation of the flow (as a function of time) into the tunnel uncertain and cumbersome. Measurements of the flow into the tunnel can, and should, certainly be made in a better way than was done at the Äspö HRL, but it should also be remembered that more detailed measurements in space and time would also have a great impact on the contractor's work and also that a dam of good quality is quite expensive.

Drawdowns

The recalculations of the drawdowns with the measured flow rate into the tunnel indicate that the drawdowns could approximately be predicted with *Model 90*. However, close to the shaft and north of the spiral the differences were rather large, mainly due to the absence, in the model, of a hydraulic conductor domain intersecting the shaft. In the *Model 90* the transmissivities of 5 conductive zones were slightly modified based on calibration of the model */Wikberg et al, 1991/*. In the *Model 95* these transmissivities were used, and according to *Table 5-4* the overall conductivity of the model seems to be a bit too high as the measured drawdown is greater than the predicted.

The hydraulic conductor domains control the drawdowns to a large extent in the modelling approach used. If the properties of the hydraulic conductor domains are changed (by calibration) the average error of the drawdown can be reduced. There will, however, remain greater or lesser individual errors. To obtain better agreement between the model and the observations there should probably be some correlation of the hydraulic conductivity within the hydraulic rock mass domains. The 'correlation length' in the simulations was about 20 m, as that was the cell size and no correlation model was used when the hydraulic conductivities was assigned to the model. There are very probably a number of conductive features larger than the cell size that are not modelled deterministically. If a reasonably good model for the correlation within the model could be defined for the spatial assignment of the hydraulic conductivity, the errors within the hydraulic rock mass domains would probably be reduced to some extent.

5.7 EVALUATION OF NUMERICAL, MATHEMATICAL TOOLS

Process

The concepts described in *Table 5-1* formed the base for the numerical groundwater flow modelling with the finite-volume code PHOENICS. Up to 1995 only steady-state simulations were performed using the PHOENICS code. It was assumed that only the concentration of salts (salinity) controls the density, and not the temperature and pressure. The salinity calculated is dependent on the advection and the dispersivity (see *Chapter 7* for details). The hydraulic conductivity was used in the simulations assuming that the dynamic viscosity of the fluid and fluid density were approximately constant within the numerical model.

Geometrical framework

Svensson /1991/ presented the principle of the way in which the hydraulic conductor domains were included in the model. The properties of cells within the numerical model intersected by a hydraulic conductor domain, approximated to a plane, are modified on the basis of the transmissivity of the hydraulic conductor domain and the intersection characteristics between the individual cell in the model and the hydraulic conductor domain. It is an efficient way of constructing a model as the geometry of the cells in the model is not dependent on the geometry of the hydraulic conductor domains.

Model development

When the predictive site-scale modelling was started around 1990 the stochastic continuum approach was chosen. During the years that followed a number of developments were made to improve the visualization of results and the calculations. Some of these developments have now been incorporated into the numerical realization of *Model 96* - as for example a new groundwater recharge algorithm */Svensson, 1995a/.* A program for conditioning the hydraulic conductivity field around the boreholes was also developed, in order to simulate in a more realistic way the dilution and water pressure in the borehole sections */Svensson, 1992/.* However, the conditioning of the conductivity field around the boreholes has so far not been incorporated into the site-scale models.

Anisotropic conditions have so far not been used in the stochastic continuum models. As anisotropic conditions may be important, the numerical models must be able to simulate such conditions.

Model approaches

International co-operation concerning modelling of groundwater flow and transport has been going on for some years at Äspö HRL. Besides the SKB, modelling teams from ANDRA, CRIEPI, PNC, Posiva and Nirex have been modelling a long-term pumping and tracer test (called LPT-2) and the drawdown in the laboratory. The major conclusion is that the general behaviour of the groundwater flow can be reproduced fairly well with all approaches based on the available data */Gustafson and Ström, 1995/.* However, the tasks have also illuminated needs for model developments and input data to the models. For example, no modelling group was able to use all interference test data for calibration purposes. More flexibility in applying boundary conditions could probably also improve the modelling in some cases. The modelling exercises have also been fruitful as they have given the modellers an opportunity to discuss modelling concepts and to test the ability to handle large data sets.

5.8 EVALUATION OF SITE INVESTIGATION METHODS

Hydraulic tests

Flow rates and drawdown/recovery are generally much better controlled during a pumping test and permit more reliable estimates compared with an air-lift test. However, in cases where both pumping tests and air-lift tests were performed the air-lift tests seem generally to give relatively reliable transmissivities of the hydraulic conductor domains.

Transient testing methods are preferred because they provide an opportunity to evaluate the flow regime and give some rationale for the choice of evaluation method. The hydraulic resistance around the borehole ('skin') that is always more or less present may also be separated from the properties of surrounding rock, which cannot be done using stationary evaluation methods. Transient tests are also useful for calibration of numerical models.

Interference tests can be rather time-consuming in planning, execution, processing of data and evaluation of data. It is very important to plan interference tests and other activities, which may cause pressure responses (for example drilling) so that they do not interfere with each other. If other tests or activities causes pressure responses, they may ruin the interference test.

During interference tests the drawdown and recovery period was generally 3+2 days. This was a good choice in terms of the influence on a large volume of rock, which is good for calibration purposes, and to reduce the negative influence earth tides may have on the evaluation of the hydraulic properties. Far away from the pumped borehole the responses are generally small and earth tides generally disturb the responses. If the measurement period is several days, the approximate trends caused by the pumping can still be seen, but if the pumping period is 0.5 - 1 day it may be impossible to judge if the response seen is caused by pumping or earth tides.

Flow-meter logging is a fast, useful and feasible method for finding hydraulic features in a borehole and obtaining a rough estimate of their transmissivities. However, in boreholes in which there is a high transmissivity in the upper part of the borehole and water with high salinity at depth in the borehole, flow-meter logging may give false results in the lower part of the borehole. The reason is that the dense, saline, water rises in the borehole up to a level where it balances the drawdown in the borehole, and the result is stagnant water in the lower part of the borehole. To obtain estimates of the hydraulic properties along the entire borehole it is therefore important to perform systematic injection or pumping tests or pumping tests within limited sections of a borehole with a double-packer system. These tests can also be performed step by step during drilling by testing the last section drilled with a single-packer system.

A few more hydraulic tests should be performed in some of the major domains compared with that done during the investigations for the Äspö HRL to better estimate the spatial distribution of transmissivity within hydraulic conductor domains.

The anisotropic conditions make it much more difficult to sample data that are useful for the analysis intended to provide a quantitative description of the anisotropic conditions. If the rock mass is anisotropic the evaluated properties will be dependent to some extent on the borehole direction (see *Figure 5-17)*. Indications of anisotropy at an early stage of an investigation programme are therefore important for the planning of the main part of the investigations and also for the evaluation of data.

The anisotropy also makes it difficult to sample data useful for estimating a correlation structure in three dimensions.

Dilution measurements and interpretation of the results

It is well known that a borehole will disturb the natural flow close to the borehole and that this has implications for the interpretation of dilution tests. The corrections applied usually assume that the direction of the natural groundwater flow is perpendicular to the borehole centre line */Halevy et al, 1967, Drost et al, 1968, Landberg J, 1982/*. An approximate relationship depending on the angle between the undisturbed flow and the borehole's longitudinal axis, borehole radius and section length in the borehole open to flow was made in *Liedholm /1991b/*. This relationship was used to transform the flow rates calculated in the numerical groundwater flow model to expected dilution rates in the boreholes.

The predicted flow rates are generally 10 to 100 times greater than the measured ones except for borehole KAS03 on northern Äspö, where predicted values were approximately as measured */Rhén et al, 1997a/*.

Dilution measurements

More reliable predictions and measurements can most probably be achieved if shorter test sections for dilution measurements are used. The test section should also preferably just straddle the hydraulic conductor domain or just be in what is considered to be a hydraulic rock mass domain. This may stand in conflict with the way in which the entire borehole is instrumented as only a limited number of test sections can be installed.

Modelling

If a hydraulic conductor domain intersects a borehole section and dominates the flow field in that section, the flux rate and direction in the hydraulic conductor domain must be the ones used together with the width of the domain to calculate the transformation factor. In many other cases it is probably difficult to define representative flux rates and flux directions in the model that are useful for estimating the flow rate in the borehole.

Generic studies were also tested to simulate a sub-model of the borehole section itself surrounded by the measured hydraulic conductivities and taking the boundary conditions from the site-scale model */Svensson, 1992/.* In this way it could be expected to be more reasonable to compare the actual measurements with the simulated flows in the borehole. This approach should be tested. In such a case no transformation is needed as it is possible to calculate the flow in the borehole section directly.

Transformation

If the impact of the borehole flow field itself and the flow in the borehole are not modelled, some correction of the filtration velocity has to be made if the filtration velocity in the numerical model is to be compared with dilution measurements. The transformation should be based on the evaluated geometrical framework and the local material properties around each borehole section but also on a thorough evaluation of the flow field around the borehole section in the groundwater flow model in order to obtain relevant parameters for the transformation. It is then likely that the transformation can be improved compared with what was achieved in the predictions, and possibly that at least the right magnitude of the flow rate can be predicted.

However, the heterogeneity will most probably cause problems in the evaluation of relevant parameters in the groundwater flow model and also in correctly describing the way in which the borehole is hydraulically connected to the formation, especially when there is a positive skin factor around the borehole. The fracture itself is very heterogenous and the measured dilution rate will depend on where the borehole intersects the fracture plane.

Even though it is evident for a number of reasons that there are difficulties in estimating the proper fluxes in the rock mass from dilution measurements, the dilution measurements are useful and a feasible way of finding out whether or not there is hydraulic communication in terms of flows and not just pressure responses.

Monitoring

The measurement intensity of the monitoring of the water pressures in space and time is judged to be mainly sufficient. However, it would have been preferable to have had somewhat more reliable measurements of the natural conditions. To some extent the natural conditions were disturbed by performance of the investigations, mainly the hydraulic tests. It also turned out that the equipment for monitoring the pressure in the boreholes was not designed for the large drawdowns close to the tunnel spiral. At the end of the excavation period several of the borehole sections close to the tunnel spiral stopped functioning. 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.

Effects of earth-tide, precipitation, barometric pressure and sea level changes on the water pressures can be seen with the measurement intensity chosen (surface holes connected to the HMS (Hydro Monitoring System): measurements every 8th minute and the value is not stored unless the change is more than 0.2 m from the latest stored value. However, a value is always stored every second hour).

The undisturbed pressure distribution along the deep cored boreholes was estimated from the transient injection tests. These absolute pressure estimates were considered uncertain but were useful for the interpretation of the chemical sampling. However, more reliable measurements of the absolute pressure during natural conditions should be made in the future. *Table 5-5* contains a summary of the usefulness of a number of methods.

Table 5-5. Judgement of the usefulness of different investigation methods for the pre-investigation phase of the Äspö HRL. ***/Almén et al, 1994/.***

Subject	**Methods**	**Usefulness**		
		Regional, Site scale	**Block scale**	**Detailed scale**
Water-bearing zones	Drilling documentation - percussion holes	2	-	-
	Drilling documentation - cored holes	2	-	-
	Air-lift tests	2	-	-
	Clean-out and pumping test of borehole	2	-	-
	Spinner or flow-metre measurement of the borehole	3	-	-
	Injection tests - 3 m packer interval	1	-	-
	Injection tests - 30 m packer interval	1	-	-
	Interference tests - test section between two packers	3	-	-
	Interference test - open borehole	2	-	-
	Interference test - open borehole - long time	3	-	-
	Other methods (geological and geophysical investigations)	3	-	-
Hydraulic conductivity	Available hydrogeological investigations in the area of interest	2	-	1
	Injection tests - 3 m packer interval	3	-	3
	Injection tests - 30 m packer interval	3	-	-
	Air-lift tests	3	-	-
	Clean-out and pumping test of borehole	3	-	-
	Interference test - open borehole	3	-	-
	Core mapping	-	-	3
Conductive structure	Injection tests - 3 m	-	3	-
Boundary conditions and pressures in the rock volume	Groundwater monitoring	3	-	-
	Borehole deviation measurements	3	-	-
Flux distribution	Dilution test	3	-	-

Very useful = 3 Useful = 2 Less useful = 1 Not applicable = -

5.9 OVERALL EVALUATION CONCERNING HYDROGEOLOGICAL CONCEPTS

5.9.1 Models

The stochastic continuum approach chosen in 1990 involved state-of-the-art modelling approaches used at that time. The model approach used in 1990 was both useful and feasible. It has been shown to be a model that is rather easy to develop and, in that respect, a good choice. The international co-operation within the Task Force on Modelling of Groundwater flow and Transport of Solutes has, however, also shown that several approaches can be used to obtain results that reproduce the pressure observations fairly well.

The model used today has an improved groundwater recharge algorithm and uses the topography to define the upper boundary. The purpose of introducing the new method is to see if it is possible to define a more robust boundary condition than, for example, constant rate, that can handle both natural conditions and large disturbance due, for example, to flow into a tunnel system (for details see *Svensson /1995a/*).

For the future, new developments are needed so that correlation models can be estimated from the field data, and also implemented in the numerical models, in order to generate the hydraulic conductivity field in a more realistic way. The hydraulic conductivity field in the models should also be conditioned against available field data, which also demands developments of the numerical models

5.9.2 Prediction and outcome approach

A summarized evaluation, based on data from a comparison between prediction and outcome */Rhén et al, 1997a/* is presented in *Table 5-6* and *Table 5-7*. The (+) sign represents the most common parameter result. Our ability to predict a certain subject (parameter) at Äspö is shown by the number of outcome results inside the predicted range. Results outside the predicted results are discussed with respect to the reason for the deviation,

The hydrogeological concepts have mostly been found to be relevant. The usefulness of individual subjects, however, can questioned.

Table 5-6. Comparison between prediction and outcome */Rhén et al, 1997a/.* **The '+' sign represents the most common parameter result.**

Subject	Site scale		Block scale		Detailed scale		Comments
	Within predicted	Outside range	Within predicted	Outside range	Within predicted	Outside range	
Major water-bearing zones							
Geometry							
Position in or close to tunnel	+						Interpretation based mainly on geology but interference tests were important for defining the NNW structures. The important zones were approximately at the predicted positions and a few corrections of others were made.
Properties							
Transmissivity	+						The most transmissive zones were within the predicted range.
Hydraulic rock mass domains							
Geometry							
Depth dependance	+						No depth dependence was predicted down to 500 m depth.
Properties							
Hydraulic conductivity	+*			+*		+*	Site scale: Outside range below the Baltic Sea south of Äspö. Close to the predicted range for depth level 200-400 m. Block scale: Two of six predictions within range. Detailed scale: Outcome both within and just outside predicted ranges. The outcome of the difference between the lithological units was as predicted.
Boundary conditions and pressures	+**						Pressures were predicted using a groundwater flow model.

* Uncertainties mainly due to anisotropic and heterogenic conditions.

** No strict ranges were given in the predictions. However, the results from simulations with two different skin factors for the tunnel are here used as prediction ranges and a judgement was made if the results were relatively close to the predicted range(=within predicted range) or not (outside range).

The predictions generally comprise both point estimates and a confidence interval at a certain confidence level. These point estimates and confidence intervals are obtained from sample properties. Predicted ranges are the results of expert judgements. The confidence level was 95% for the confidence limits of the point estimate. 'Range' in the table above may be the confidence limits or the ranges based on expert judgements.

Table 5-7. Comparison between predictions and outcomes ***/Rhén et al, 1997a/.*** **The '+' sign represents the most common parameter result.**

Subject	Site scale		Block scale		Detailed scale		Comments
	Within predicted	Outside range	Within predicted	Outside range	Within predicted	Outside range	
Flow into the tunnel	(+)						Fairly close to predictions. The flow rate is more dependent on the grouting in the tunnel than on the hydraulic properties of the rock mass and zones.
Flux distribution		+					The directions of the predicted changes of flux rates in the borehole sections are generally as the measured ones. Predicted rates are generally much larger than those observed. Long borehole sections for measurements are probably one of the reasons.
Conductive structures			+*				The distance between hydraulic conductors along boreholes with a transmissivity greater than a specified value was predicted.
Flow in conductive structures			+**				Flow distribution around the tunnel periphery was predicted.
Pressure around the tunnel			+			+	The variability in the measured pressure is large.
Point leakage							
Wet tunnel area					+**		Wet tunnel area by rock type
Inflow characteristics					+**		Characteristics: Flows, drips or moisture to sporadic drips.
Inflow types						+**	Types: Bolthole, node, extensive, point or diffusive.

* Uncertainties mainly due to anisotropic and heterogenic conditions.

** No strict ranges were given in the predictions. However, the results from simulations with two different skin factors for the tunnel are here used as prediction ranges and a judgement is made if the results are relatively close to the predicted range(=within predicted range) or not (outside range).

The predictions generally comprise both point estimates and a confidence interval at a certain confidence level. These point estimates and confidence intervals are obtained from sample properties. Predicted ranges are expert judgement. The confidence level was 95% for the confidence limits of the point estimate. 'Range' in the table above may be the confidence limits or the ranges based on expert judgements.

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 coreholes were less extensive in the uppermost 100 m of the boreholes and due to this the interpretation became more difficult and uncertain. Standardized investigations should be performed in a consistent way in the entire borehole using a few methods. Specially designed tests may then be performed in parts of the borehole where a hydraulic conductor domain is interpreted as intersecting the borehole.

It is also valuable to have a good three-dimensional CAD system in which results from the investigations, the geological and hydrogeological model can be visualized during the investigations. An effective tool was not available during the pre-investigation and construction phases of the tunnel.

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. It is judged that the effective values of the hydraulic conductivity of the rock mass domains between the major conductor domains or for lithological domains can be predicted if several boreholes penetrate the volume to be predicted. Extrapolation of results to rock volumes outside the investigated volume may be unreliable, at least if for geological reasons it can be expected that the fracture characteristics are different from those in the investigated volume.

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 heterogenous on a large scale. Anisotropic conditions will also make it more difficult to perform relevant tests and evaluate the properties. There is a scale dependency that has been handled using data from a number of boreholes, with tests performed over different lengths in them, to formulate an empirical relationship. Efforts should be made to continue performing tests in a systematic way so that at least two test scales, besides tests in which the entire borehole is pumped, are used as long as no reliable method for scaling is available. More efforts should also be made to develop a somewhat more realistic spatial correlation model for the hydraulic conductivity.

Methods

It is important to perform tests at different scales systematically in the boreholes, both for scale relationships but also for the 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 larger scale interference tests both for defining hydraulic conductor domains and for calibrating and obtaining test cases for numerical groundwater models.

5.9.3 New knowledge from the tunnel

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. */Rhén et al, 1997b/.*

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 */Rhén et al, 1997b/.* The data were also used to obtain rough estimates of the hydraulic resistance around the tunnel due to grouting or effects of the disturbed zone.

The investigation along the tunnel also 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 transmissivities for the zones.

5.9.4 Conclusions

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

- To construct a reliable model it is important to perform tests on different scales systematically in the boreholes, 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. It is also important to have a good three-dimensional CAD system in which results from the investigations, the geological and the hydrogeological model can be visualized during the investigations.

- A site that is heterogenous 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. For example, new developments are needed so that spatial correlation models set up can be used to generate the hydraulic conductivity field in a more realistic way and also to condition the hydraulic conductivity field against field data. Developments are needed to achieve more efficient handling of input data and calibrations and also to obtain better visualization of the results.

- Interference tests can be rather time-consuming in planning, execution, processing of data and evaluation of data. It is very important to plan interference tests and other activities, which may cause pressure responses (for example drilling) so that they do not interfere with each other. If other tests or activities causes pressure responses, they may ruin the interference test.

- Measurements and evaluation methodologies of dilution rates should be further studied to obtain more confidence in how to calculate more reliable flow rates in the rock mass from the dilution rates.

- The measurement intensity of the monitoring of the water pressures in space and time is judged to be mainly sufficient. However, it would have been preferable to have had somewhat more reliable measurements of the natural conditions. To some extent the natural conditions were disturbed by performance of the investigations, mainly the hydraulic tests.

- More reliable measurements of the absolute pressures along the boreholes at natural (undisturbed) conditions should also be made to provide better possibilities for interpretation of the water chemical sampling, especially in open boreholes.

6 EVALUATION OF MODELS FOR GROUNDWATER CHEMISTRY

6.1 INTRODUCTION

The purpose of the groundwater chemical investigations and descriptions is to give a view of the possible variations and the long-term stability of the observed concentrations of elements and other properties, major ions, trace elements etc. which are important for the construction and performance and safety assessment of a nuclear waste repository. A second purpose, at Äspö, is to provide a description of the groundwater flow system evolution in the past.

The hydrochemistry model is a description of the groundwater composition in the investigated rock volumes, focusing on the southern part of Äspö island. The description is related to the water in the interconnected fracture system, consisting of the major and minor water-conducting fracture zones and conductive fractures. Groundwater samples are collected from these boreholes on different occasions (see *Almén et al /1994/*). The groundwater chemistry of the isolated water in the rock matrix is not included. The reason for this limitation is that hydrochemical investigations, carried out through boreholes, can only focus on the high-conductivity borehole sections. However, a pilot study of the water in the low-conductivity rock mass is presented in model *Report 5* in this series */Rhén et al, 1997b/.* The results indicate only minor differences in composition compared with the water sampled in the high-conductivity borehole sections. Further studies are planned.

The models for groundwater chemistry are presented in detail in *Report 5* in this series */Rhén et al, 1997b/* as an over-all hydrochemical model of Äspö. The description of the model includes the processes considered to be the most important for the observed groundwater composition. *Table 6-1* includes the different concepts under which the processes are discussed. The structure of the table is the same for all the disciplines, geology, mechanical stability, hydrogeology and chemistry. From a hydrochemical point of view, it is more important to describe some parts of the concepts than others. Introductory comments to *Table 6-1* are:

- The mixing of different end-members (original groundwater types) is a physical process taking place both at present and in the past. This process is governed by the hydraulic conditions, i.e. head and transmissivity at present and in the past.

- The mixing process is closely linked to the geometry of the hydraulic structures (water-conducting fracture zones and fractures) whereas for the other processes there are no strict relations to the geometry of water conductors.

- Groundwater/rock interaction includes all processes affecting the groundwater chemistry, specifically calcite saturation, redox and biological processes, which have the greatest influence on the groundwater composition.
- Groundwater properties (i.e. concentrations of constituents) are affected differently by different processes.
- Spatial assignment methods are related to the prediction of groundwater chemical properties in the tunnel on the basis of pre-investigation data and models.

Table 6-1. Condensed description of the components of the hydrochemical models of the Äspö site.

HYDROCHEMICAL MODELS OF THE ÄSPÖ SITE

Scope:
Present and past groundwater composition in fracture zones and hydraulically interconnected single fractures. (does not include water isolated in the rock matrix, e.g. fluid inclusions.)

Process description:
Mixing of water with different origin and composition
Groundwater/rock interaction: Calcite saturation, redox controlling processes, biological activity, ion exchange.

CONCEPTS

Geometrical framework:
Mixing in deterministic fracture zones defined as planes in the rock volume.
Distribution of groundwater types in the rock mass.

Groundwater properties:
Concentrations of Na, Ca, K, Mg, Cl, SO_4, HCO_3, Fe, HS. The master variables pH, Eh, and contents of TOC (Total Organic Carbon), dissolved gases, microbes, isotopes.

Spatial assignment method:
The following alternative methods have been used:

- Traditional hydro-geochemical evaluation methods,
- Multivariate (Principal component) analyses,
- Linear regression,
- Kriging,
- Neural Networks

Boundary conditions:
Conditions affecting the groundwater chemistry at present and in the past, i.e. to identify end-members and reference waters.

Output parameters:
Mixing proportions of reference waters and end-members,
Saturation index, equilibrium concentrations,
Data on groundwater properties and residence time

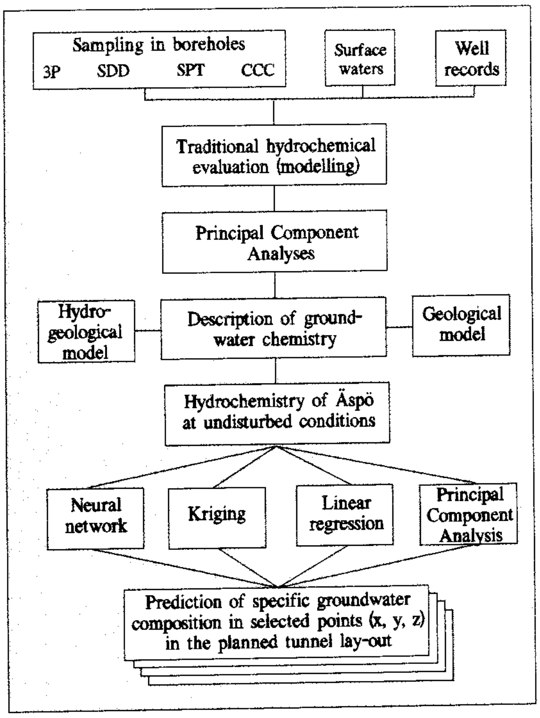


Figure 6-1. *A schematic presentation of the methods used for the hydrochemical investigations. '3P' , 'SDD', 'SPT', 'CCC' and 'Surface Waters' complemented by well records comprise the sample collection and chemical analysis made by the Äspö HRL project, see Table 6-2.*

The pre-investigation methodology for characterization and the groundwater chemistry is presented in *Figure 6-1*. Discussion about the pre-investigation methods is presented in *Section 6.2.1*.

During the tunnel construction phase groundwater samples were collected and analysed mainly to provide the data necessary for comparison with the predictions and to give a more detailed description of the different processes which affects the groundwater composition.

6.2 HYDROCHEMICAL MODEL

6.2.1 Groundwater chemical properties

Concentrations of Na, Ca, K, Mg, Si, Cl, SO_4, HCO_3, Fe, HS, pH, Eh, TOC (total organic content) or DOC (dissolved organic carbon), dissolved gases, microbes, isotopes are the properties of the groundwater which are included in the hydrochemical description of Äspö. Some of them are essential for the safety assessment of a deep repository, whereas some are important for understanding the way in which the groundwater chemistry has evolved in the past. This may be almost as important, since understanding the past is the key to understanding the future. The present model includes a palaeo-hydrological view of the conditions which have influenced the groundwater chemistry since the latest glaciation. We might assume these conditions to be repeated after a future glaciation as well, and in such a case expect similar influences on the groundwater chemistry after the next glaciation.

The concentrations of major constituents Na, K, Ca, Mg, Cl, SO_4, HCO_3, Fe, HS, and pH and Eh largely define the character of the groundwater chemistry. However, for performance assessment calculations the amount of organic matter, TOC, and especially the fractions of fulvic and humic acids are needed as well as the concentrations and types of microbes and colloids. Nitrite, nitrate and ammonium concentrations were mostly below the level of detection (of order ppb). These elements were only rarely measured */Smellie and Laaksoharju, 1992/.*

Most information on groundwater chemistry was collected from sampling of the deep cored holes. The different sampling procedures are all listed in *Table 6-2.* The analytical data are presented in *Appendix 2.*

As such the drilling might affect the hydrochemistry severely by causing an artificial mixing which could be difficult to separate from the natural mixing situation. This disturbance can vary from one sampling location to another depending on the technical conditions during drilling and on the hydraulic situation. An empirical classification of the water-conducting fracture zones has been made to handle the risk of disturbances:

- ‘Highly conductive’ (transmissive) - borehole sections (zones) with a hydraulic transmissivity above 10^{-5} m^2/s, are generally contaminated by drilling water. However, a carefully planned hydrochemical characterization in conjunction with hydraulic pumping tests has given valuable information on the origin and mixing of different groundwater types. The relatively large pumping rate gives an opportunity to observe possible transients in the composition due to variations in the proportions of different water types.

- ‘Conductive’ - borehole sections with a hydraulic transmissivity of 10^{-5} - 10^{-8} m^2/s, are optimal for detailed and careful hydrochemical characterization. The mobile field laboratory unit was constructed specially for this purpose.

- ‘Low conductivity’ sections - transmissivity below 10^{-8} m^2/s cannot be sampled as part of a surface based site investigation programme, simply because it would be too time-consuming to extract a large enough volume of water from the low-conductivity borehole sections. Other methods like pore extraction of core samples might be more appropriate.

Table 6-2. Overview of sampling and analyses programme.

Constituents	3P	SDD	SPT	CCC	Tunnel 1	Tunnel 2
pH	3	-	1	1	0	0
Eh	-	-	-	1	-	4
Sodium	2	3	1	1	-	0
Potassium	2	3	1	1	-	0
Calcium	2	3	1	1	-	0
Magnesium	2	3	1	1	-	0
Chloride	2	3	1	1	0	0
Bicarbonate	2	3	1	1	0	0
Sulphate	2	3	1	1	-	0
Silica	-	3	1	1	-	0
Iron (total)	-	-	1	1	-	0
Iron(II)	-	-	-	1	-	0
Manganese	-	-	1	1	-	0
Strontium	-	-	2	2	-	0
Lithium	-	-	3	3	-	0
Sulphide	-	-	1	1	-	4
Bromide	-	-	3	3	-	4
DOC	-	-	2	2	-	4
Colloids	-	-	-	4	-	-
Uranium	-	-	3	3	-	4
Uranium isotopes	-	-	3	3	-	4
Oxygen-18	3	-	2	2	5	0
Deuterium	3	-	2	2	5	0
Carbon-14	-	-	3	3	-	-
Carbon-13	-	-	-	-	-	4
Strontium-87	-	-	-	-	-	4
Sulphur-34	-	-	3	3	-	4
Dissolved gas	-	-	-	3	-	4

3P = sampling of shallow, percussion drilling holes, pumping for 12 hours
SDD = sampling during drilling of deep, cored holes, pumping for a minimum of 1 hour
SPT = sampling during pumping tests, pumping for three days
CCC = complete chemical characterization in separate campaigns, pumping for ten days
Tunnel 1 = sampling at the end of the probe hole drilling in the tunnel
Tunnel 2 = repeated sampling in the selected probe holes = the constituent has not been analysed
0 = analyses are made each time a sample is collected
1 = analyses are made daily during a pumping campaign lasting for at least three days
2 = samples are collected for analyses on a few occasions during a pumping period
3 = samples are collected at the end of a pumping period
4 = samples are analysed only when some specific questions arise
5 = stored samples are analysed afterwards if specific needs arise

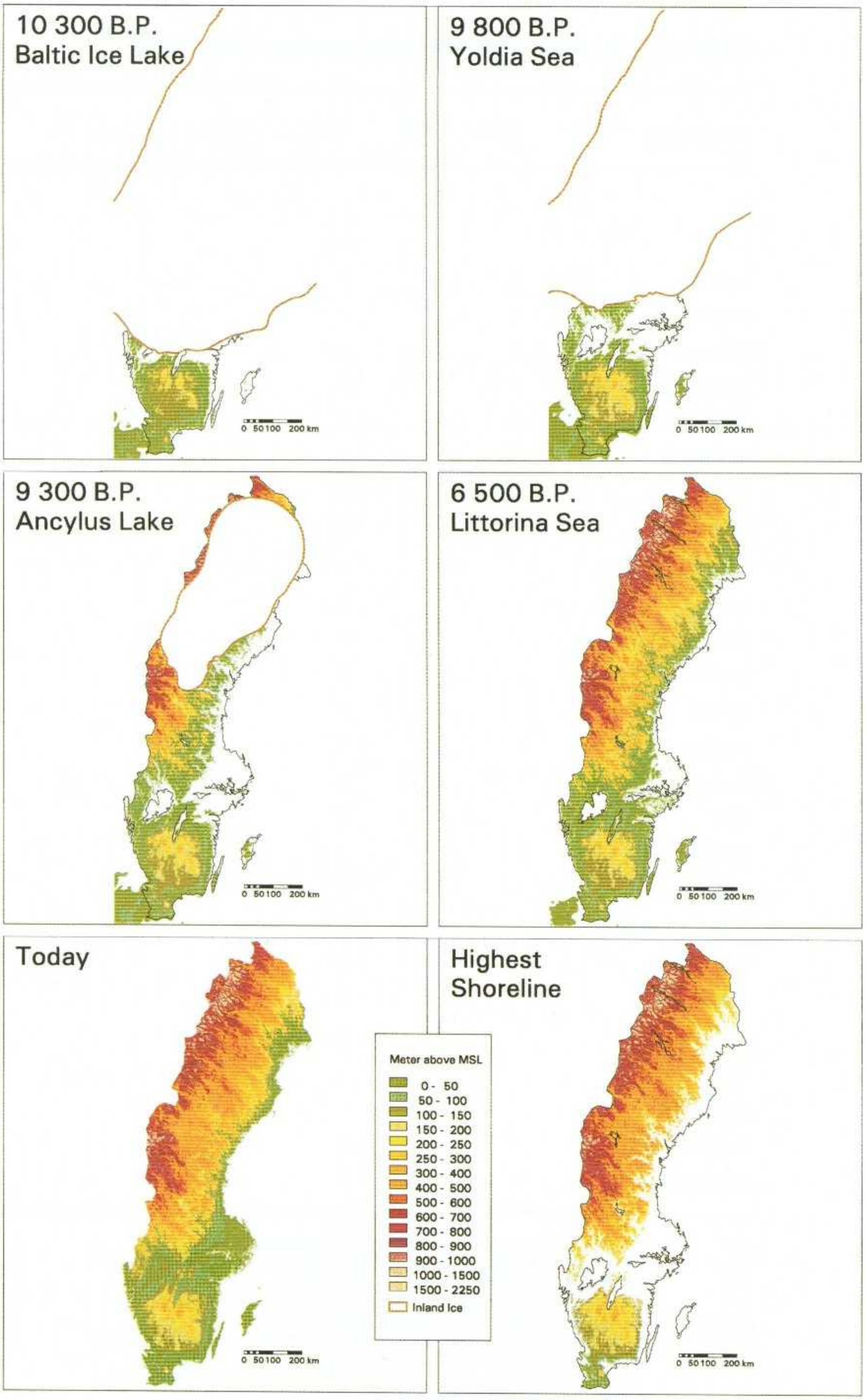


Figure 6-2. *The different evolutionary stages of the Baltic Sea after the most recent glaciation and a picture of the previous highest coastline. The pictures were produced from SKB's Geographic Information System. /SKB, 1995/.*

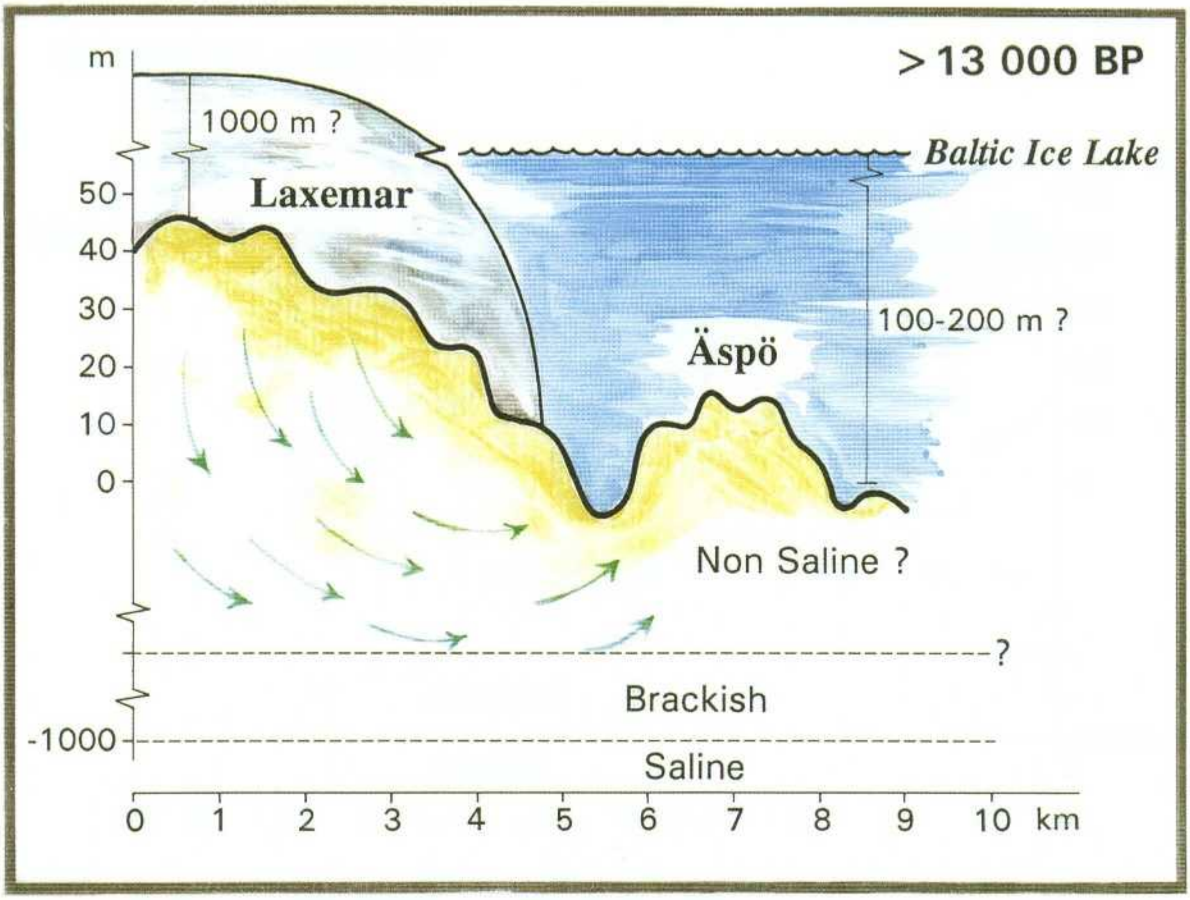


Figure 6-3. A post-glacial scenario at Laxemar and Äspö. Possible flow lines from the hydraulically driven injection of glacial melt-water into the basement.

6.2.2 The groundwater history of the Äspö-Laxemar area

The groundwater in the Äspö area reflect pre-glacial, glacial and post glacial conditions. There has been a number of episodes during which the groundwater has been largely affected regarding both flow and chemistry. The deglaciation and subsequent land rise is the most important recent event in the Äspö groundwater history. *Figure 6-2* shows the coast line of Sweden at the different stages of the Baltic Sea during its shifting between freshwater lakes and brackish seas since the last glaciation.

When the continental ice was melting and retreating, glacial melt-water was injected into the basement, *(Figure 6-3)*. The depth to which the melt-water reached is largely unknown. Groundwater flow models suggest that under hydraulic gradients caused by a thick ice cover the melt-water could be pressed to a depths of more than 1000 m at Äspö */Svensson, 1996/*. The present hydrochemical data cannot tell whether or not this has been the case. There is a clear indication of a "cold" water signature down to a depth of 1000 m which implies that glacial water is present at that depth. However, the water at 1000 m has such a high salinity that it can hardly be explained as a result of mixing of glacial meltwater and brine as a two component system. Therefore it seems

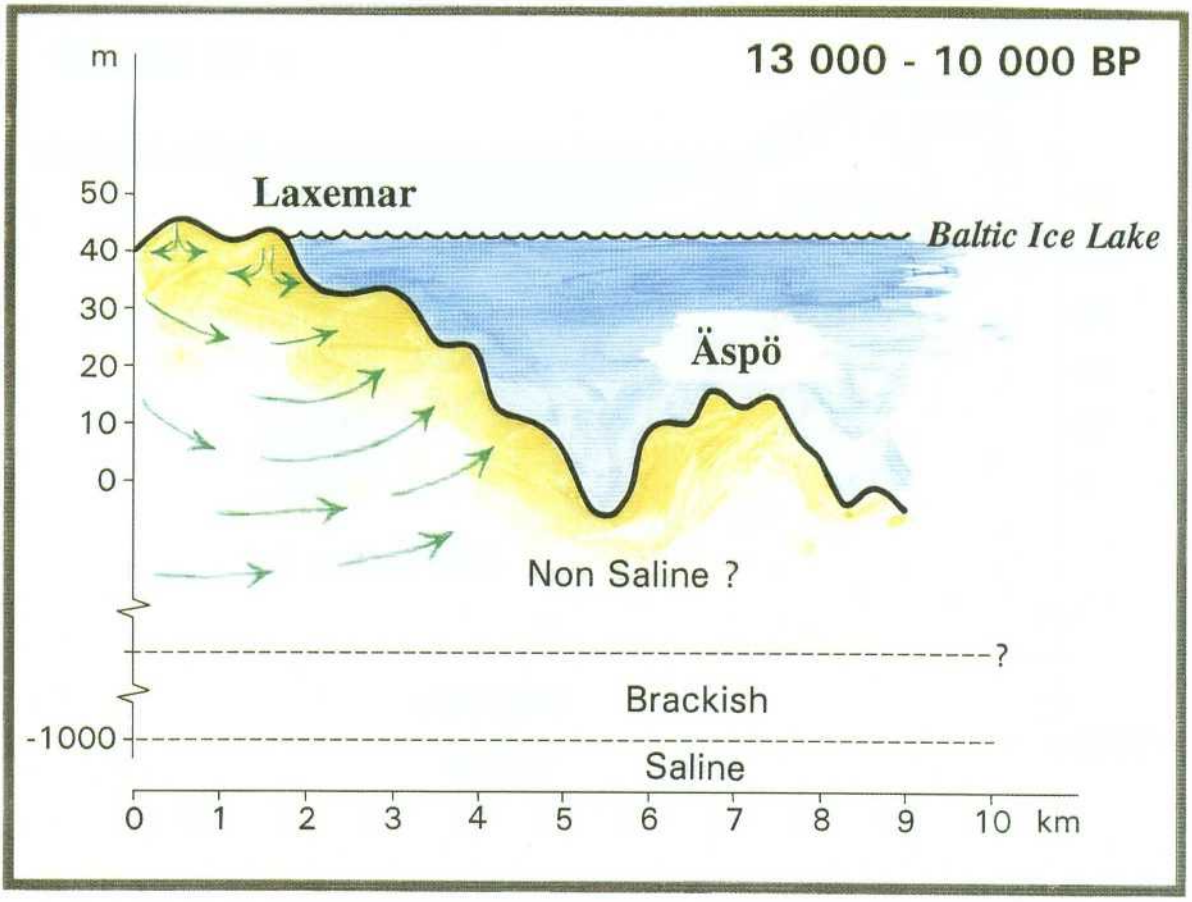


Figure 6-4. *A post-glacial scenario at Laxemar and Äspö. Possible flow lines from the hydraulic head at Laxemar. The Baltic Ice Lake covered the Äspö island.*

more likely that the glacial water at depths of a 1000 metres is resulting from some previous glaciation or that glacial melt water could also be drawn down via pumping. The effects of meltwater from the latest glaciation is observed to a depth of 200-300 m.

The first stage of the Baltic Sea, known as the Baltic Ice Lake, started to form about 13 000 years ago. 10000 years ago the Baltic Ice Lake covered Äspö *(Figure 6-4)*. The fresh water did not affect the groundwater in the basement since the density was similar and there was no hydraulic head difference when the island was under water. Far to the west, the Laxemar area rose above the water level.

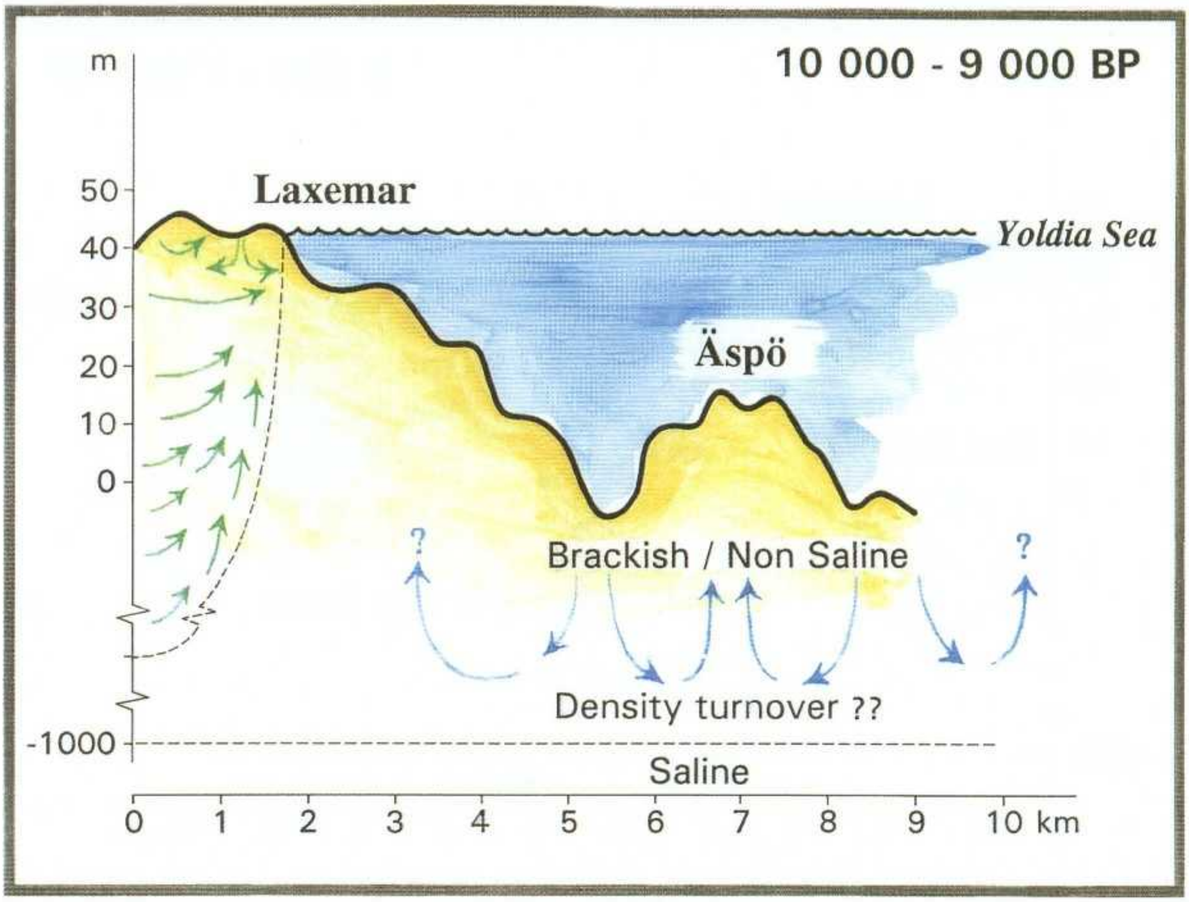


Figure 6-5. A post-glacial scenario at Laxemar and Äspö during the Yoldia Sea stage.

During the next phase the Yoldia Sea (10000-9000 B P) covered the island. The brackish-marine water could have affected the more conductive upper parts of the basement by density-driven turnover (buoyancy flow), as shown in *Figure 6-5*. The Yoldia Sea stage was short compared with the other stages and the influence on the groundwater system could have been insignificant.

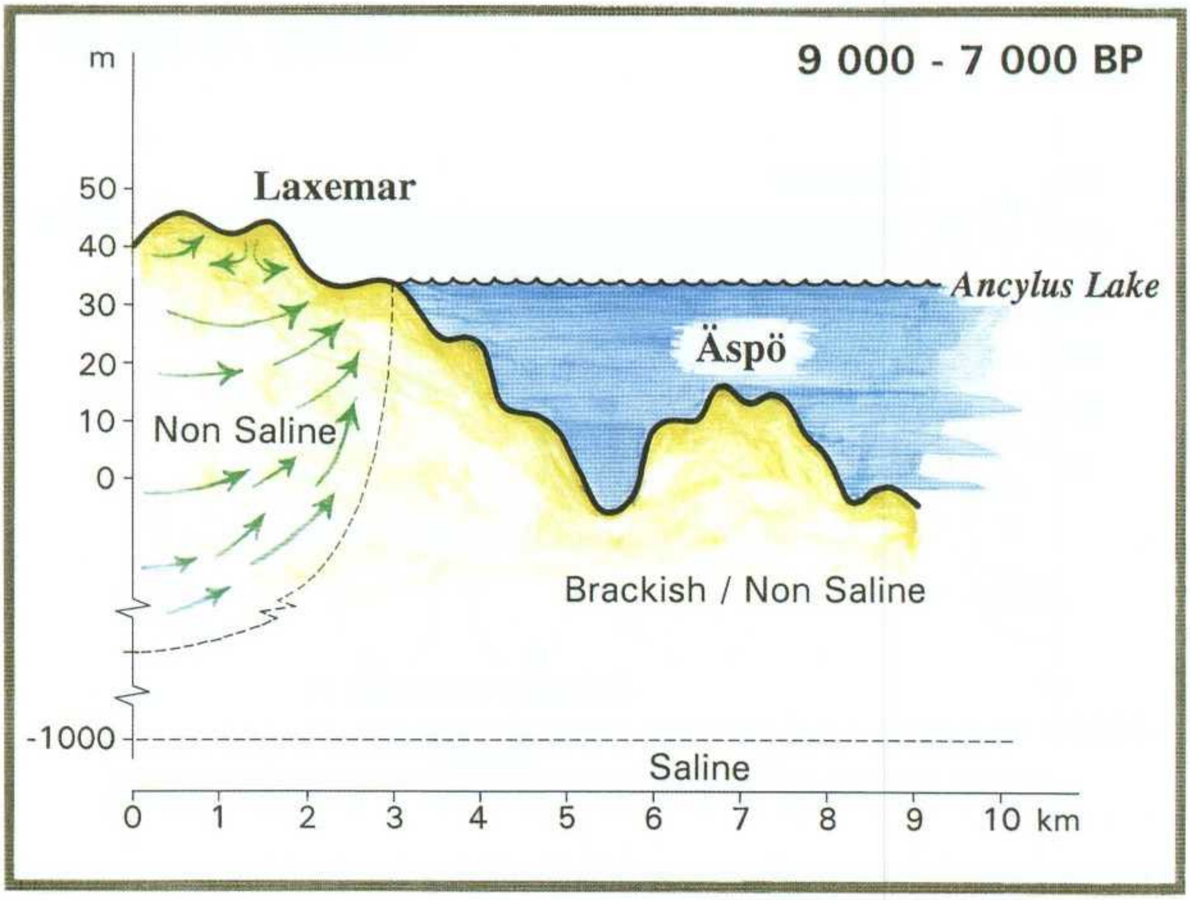


Figure 6-6. A post-glacial scenario at Laxemar and Äspö during the Ancylus Lake stage.

The Ancylus Lake (9000-7000 B P), which was a freshwater lake, did not influence the water in the basement of Äspö. At Laxemar the recharge and discharge controlled by the topography affected the areas above the water level *(Figure 6-6)*. The next stage was the Litorina (7000-2000 B P) Sea. Density-driven turnover is believed to be an important process during this period. The glacial water was replaced and mixed with the sea water *(Figure 6-7)*. In the Baltic Shield area the highly saline coastal groundwaters are only found below the highest level of the post-glacial Litorina Sea since the density-driven turnover was probably an important process during this stage.

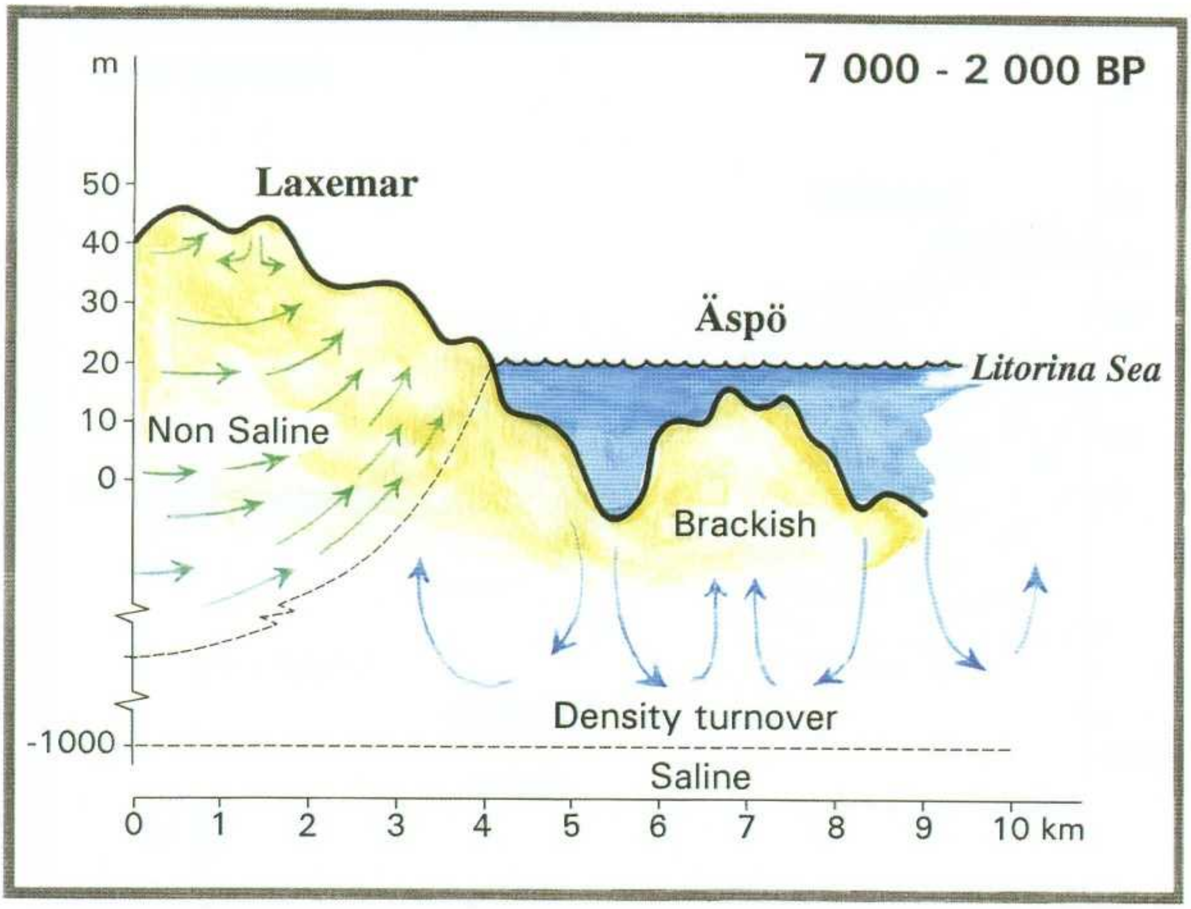


Figure 6-7. *A possible post-glacial scenario at Laxemar and Äspö. Possible flow lines, density-driven turnover, non-saline, brackish and saline water interfaces are shown. Litorina Sea stage.*

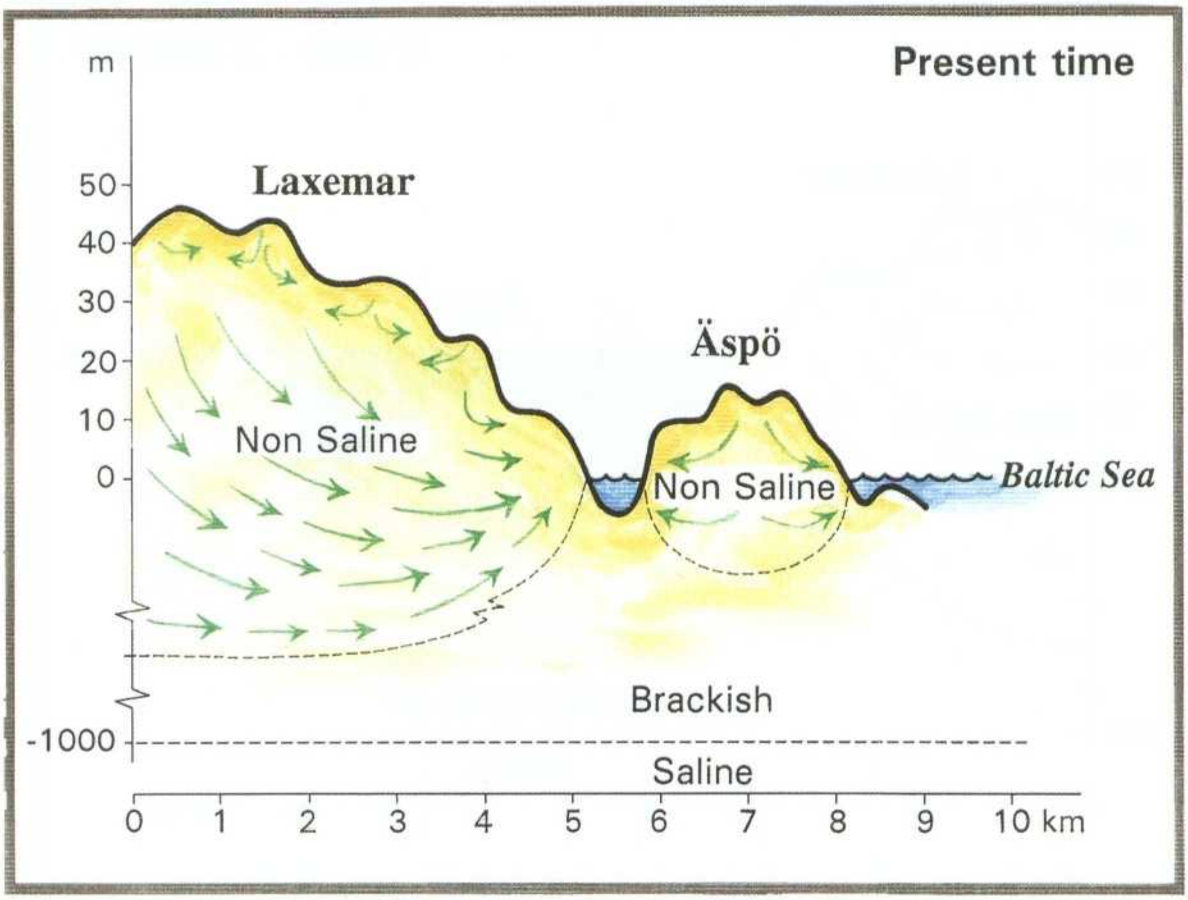


Figure 6-8. *Present day situation at Laxemar and Äspö.*

Äspö island rose above the sea level some 4000 B P. A meteoric water aquifer started to form which created hydraulic head differences and started to wash the sea water out of the more shallow parts of the basement *(Figure 6-8).* Regional flow from the mainland could have started to affect the water composition. The saline waters at depth were probably not affected by the post-glacial events *(Figure 6-4--6-7).* Traces of deglaciation in more shallow groundwaters should be detectable in the groundwater composition.

6.2.3 Present day models

The model from the pre-investigation was used to make the detailed predictions of concentrations of the main constituents to be observed during tunnel construction (see *Section 6.3).*

The isotopes, both radiogenic and stable, were used to evaluate the pre-history of the groundwater. Due to the scarcity of the data from pre-investigations it was not possible to predict the isotopic signatures of the groundwater. During the construction phase */Wallin and Peterman, 1994/* the knowledge of end-member signatures and background levels have increased. These are described in detail in *Rhén et al /1997b/.* The combination of several isotopic methods has provided the means to tackle the history of the groundwater in a systematic way. So far the events occurring after the latest glaciation have been resolved and these data have been of the outmost importance for the identification of the end-members used to construct *Model 96.*

An illustration of the models based on the data from pre-investigations and the data from the tunnel construction phase are given in *Figure 6-9*. The corresponding salinity distribution is presented in *Figure 6-10* and *6-11*. The differences in salinity distribution are due to the effects caused by the tunnel drawdown. The biological and redox conditions are not presented since they are considered to be evenly distributed in the rock mass.

The *Model 96*, developed during the construction phase, is more developed and quantitative than *Model 90* from the pre-investigation phase. In *Figure 6-9* the presentation is made in such a way that the models can be compared, but it must be realized that the figure is only an illustration of the models. *Model 90* groups the groundwater observations into four classes based on principal component analyses. The *Model 96* defines the end-members, reference waters and mixing proportions of the reference waters. This is a comprehensive modelling work which is described in detail in *Report 5* of this series */Rhén et al, 1997b/.* In *Figure 6-9* the dominating reference waters are qualitatively related to the statistically defined classes of the previous model.

A consistent picture was obtained by ^{2}H, ^{3}H, ^{18}O, ^{13}C, ^{14}C, ^{87}Sr, ^{34}S and ^{36}Cl analyses which were made on different occasions during tunnel construction. There are a few additional isotopic methods, $^{36}Ar/^{40}Ar$ and ^{85}Kr which might be useful for differentiating between the effects of the latest and previous glaciations. So far these methods have not been employed on Äspö groundwater samples.

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. This knowledge is then useful for defining the possible gradual evolution in the future.

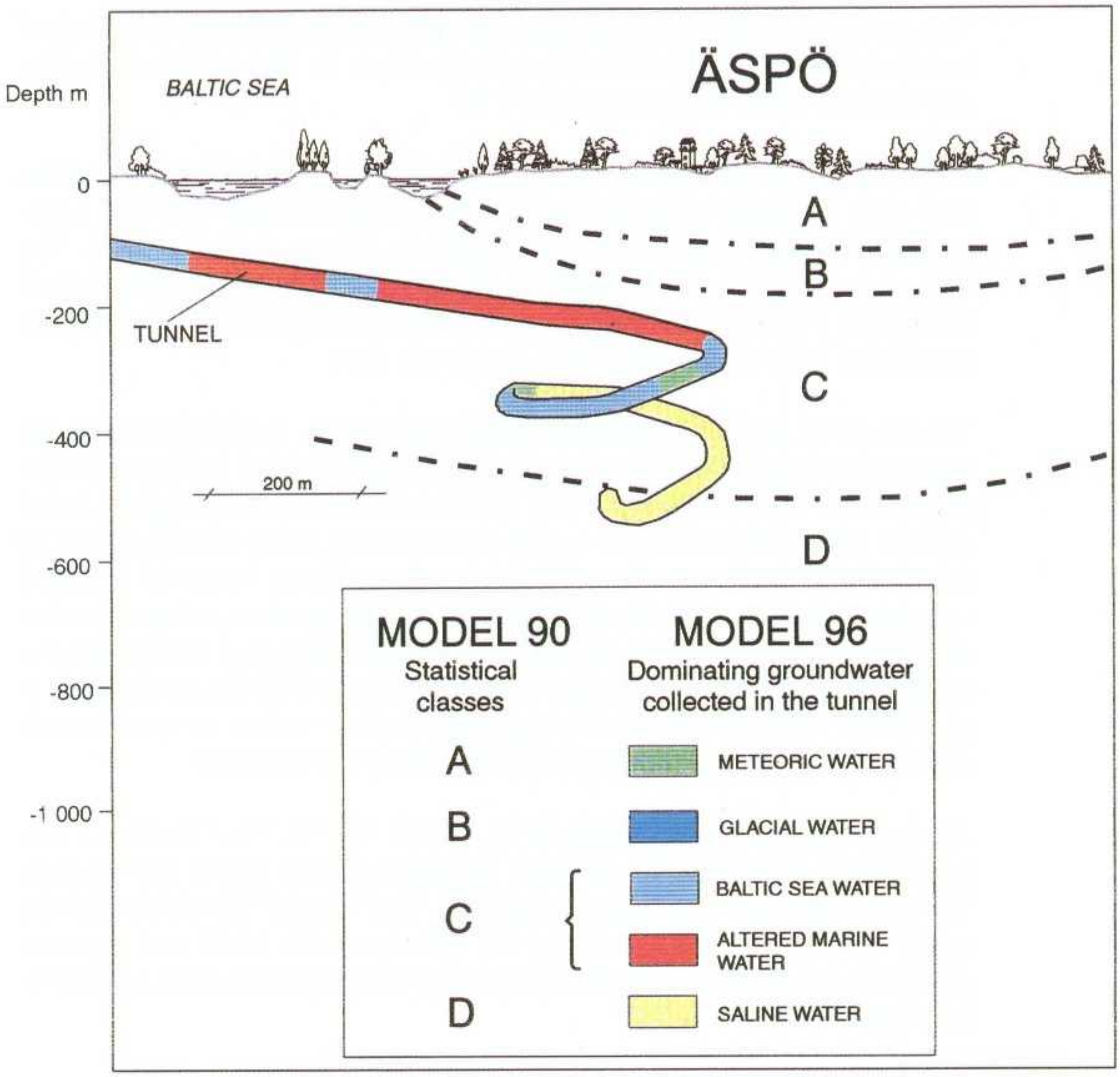


Figure 6-9. *Illustration of Model 90 based on data from the pre-investigations and Model 96 which also involves the data collected during the tunnel construction phase. Model 90 defines 4 four classes based on statistical treatment of the data, whereas Model 96 is based on identified end-members and selected reference waters and the mixing proportions of these waters (see Rhén et al /1997b/).*

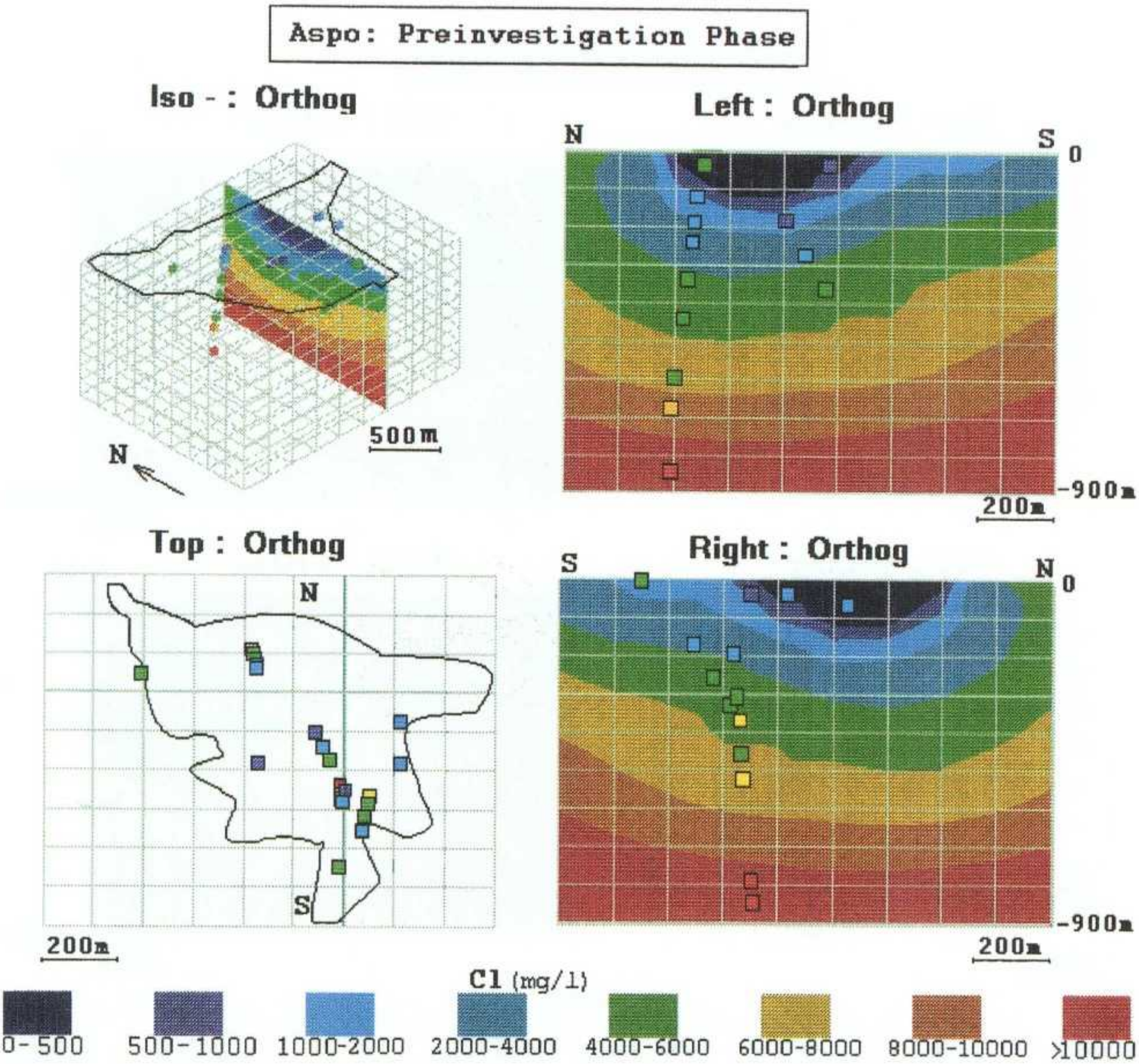


***Figure 6-10**. The salinity distribution presented as the chloride concentration under the undisturbed conditions prior to excavation. The sampling locations are marked in the figure. (Total salinity = 1.7 times the chloride concentration).*

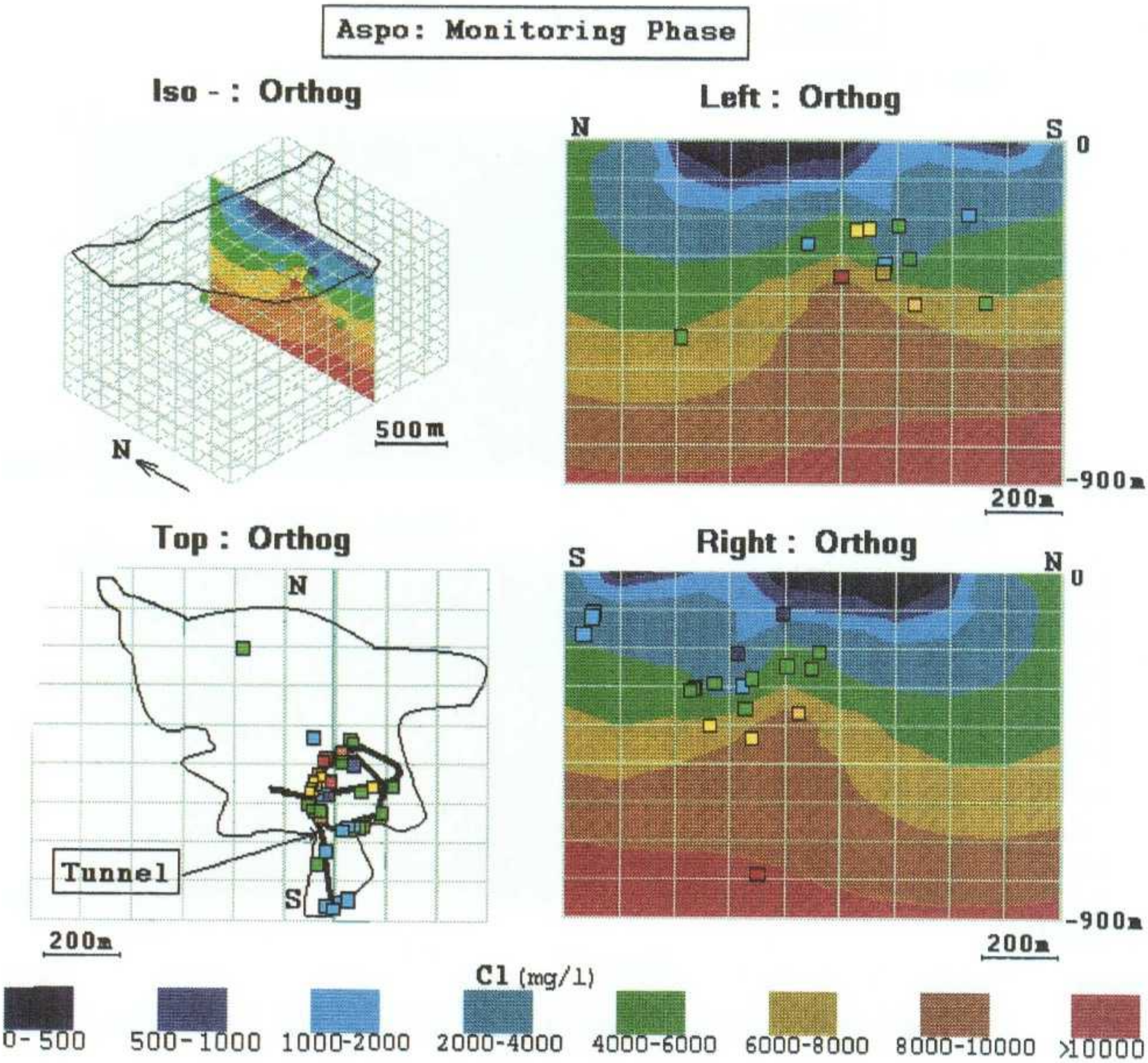


Figure 6-11. The salinity distribution presented as the chloride concentration under the disturbed conditions after construction. The sampling locations are marked in the figure. (Total salinity = 1.7 times the chloride concentration).

6.2.4 The mixing process

There are two main causes for the mixing. One is the disturbance caused by the borehole by short-circuiting the different water conducting fracture systems, the other one is the mixing which has taken place in the past due to varying hydraulic driving forces which has driven the groundwater flow in different directions. In the evaluation work, the mixing caused by the borehole is considered a disturbance which is taken into account and corrected for. The remaining mixing proportions of different water types is then described as the result of varying groundwater flow conditions. The mixing process has been in depth assessed by *Laaksoharju and Skårman /1995/* and by *Laaksoharju and Wallin, /1997/.*

Mixing is considered to be the main reason for the observed hydrochemical situation. It is because of mixing that the different end-members (=original groundwater types) identified in the hydrochemical system are not isolated to some specific volumes of the rock mass. The mixing has probably been most effective during episodes of glacial ice melting and intrusion of sea water and subsequent land uplift. The effects of such episodes affecting the Äspö groundwater system after the last glaciation have been well established, while the conditions prevailing before and during the last glaciation is largely unknown.

The end-members identified in the mixing modelling are largely the result of the episodic events. It should be noted that the further back in time the events occurred, the more uncertain are the definitions of the end members. It is strictly speaking not possible (nor perhaps even necessary) to define the end-member of the Brine. It has evidently been isolated from the atmosphere for more than one million years */Louvat, Michelot and Aranyossy in Laaksoharju and Wallin, 1997/* but it might still be involved in a regional flow system */Voss and Andersson, 1993/.*

A detailed description of the evaluation and definitions of end-members and reference waters is found in *Report 5* in this series */Rhén et al, 1997b/.* A short description is given below:

- **Glacial meltwater** end-member which is represented by the glacial reference water in the calculations. The glacial reference water consists of roughly 50% glacial meltwater.
- **Brine** is represented by the *most saline* water encountered at the bottom of the 1700 m deep KLX02 borehole at Laxemar. Saline water is, thus, a reference water, see *Figure 6-9.*
- **Baltic Sea water** is a reference water. The end-member to the present day Baltic Sea water is the preceding **Litorina sea water.**
- **Altered marine water** is a reference water which is an *original Baltic Sea water with a modified composition due to bacterial activity.*

- **Meteoric water** is the reference water which has the composition and isotopic signature of modern precipitation.

The Brine reference water has a salinity of 80 g/l which is slightly below the defined limit of 100 g/l TDS */Davis, 1964/.*

Table 6-3 summarizes the mixing proportions found in the identified fracture zones in the tunnel. The reference waters selected for the mixing calculations can vary depending on the purpose of the calculations. The ones selected to represent the Äspö site in *Figure 6-9* are slightly different from the ones selected to calculate the proportion in *Table 6-3*. The data of *Table 6-3* is graphically presented in *Figure 6-12*.

It may be seen that there are clear differences in the mixing proportions related to whether the sampling point is located under the island of Äspö or under the sea. The fracture zone NNW-4 has a large proportion of sea water from the interconnection to NE-1, through which the sea water reaches NNW-4. NE-2 has a smaller proportion of sea water than the other zones.

Table 6-3. Mixing proportions of the waters in the identified fracture zones in the tunnel. The location of the fracture zones can be found in *Figures 3-13* and *3.19*. Detailed descriptions of the fracture zones and mixing modelling are given in *Rhén et al /1997b/*. In this table the altered marine water and Baltic Sea water have been summed up to represent water of marine origin. The fracture zones NE-2 and NNW-4 are encountered at several positions in the tunnel. Bold figures indicate the largest proportion of the dominating water type of each fracture zone.

Fracture zone	Time since start of construction (days)	Proportions of the different reference waters (%):				Sampling point (borehole)
		Meteoric	Baltic Sea	Glacial	Brine	
NE-4	350	29	44	17	11	SA850B
	750	23	66	9	2	SA813B
	1150	20	68	9	3	
	1350	23	**69**	7	1	
NE-3	350	15	76	6	3	SA976B
	550	13	**77**	6	3	SA1062B
	750	14	75	8	4	SA1062B
	950	18	67	11	4	SA958B
	1150	18	66	12	4	
	1350	20	70	8	2	
NE-1	550	30	43	17	10	SA1342B
	750	25	56	15	4	SA1327B
	950	20	71	7	2	SA1229A
	1150	17	68	11	4	HA1327B
	1350	16	**76**	6	2	SA1229A
EW-3	750	29	43	23	6	SA1420A
	950	25	61	11	3	
	1150	19	**68**	10	3	
	1350	25	64	9	2	
NE-2,1	750	10	12	**66**	12	SA1614B
	950	15	18	50	17	
	1150	21	26	39	14	
	1350	26	31	30	13	
NE-2,2	750	19	23	**45**	13	SA1828B
	950	22	27	35	16	
	1150	23	28	33	16	
	1350	32	36	19	13	
NE-2,3	1150	15	21	**46**	18	SA2583A
	1350	16	20	46	18	
NNW-4,1	950	30	**38**	17	15	SA2074A
	1150	29	42	17	12	
	1350	30	41	18	11	
NNW-4,2	950	31	38	18	13	SA2109B
	1150	16	**64**	14	6	SA2142A
	1350	26	47	15	12	SA2175B
NNW-4,3	1350	16	20	**45**	19	KF3191F

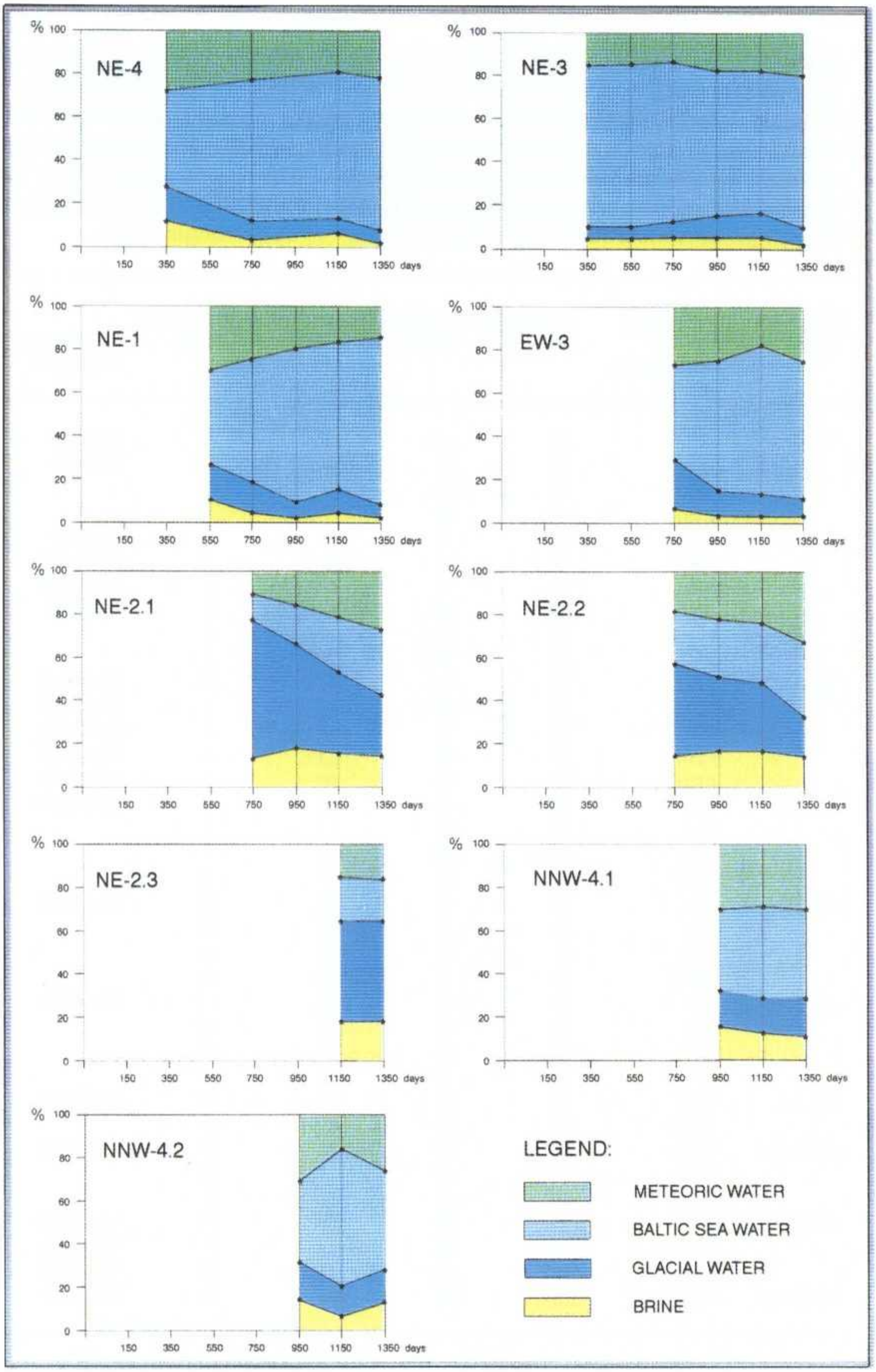


Figure 6-12. *Mixing proportions of the waters in the identified fracture zones in the tunnel. The location of the fracture zones can be found in Figures 3-13 and 3.19. The time axis shows the time since start of construction.*

6.2.5 Calcite dissolution and precipitation

Calcite reactions are among the few between solid phases and dissolved components that are rapid. The calcite system is controlled by the calcium and bicarbonate concentrations together with the pH value and solid calcite. The partial pressure of carbon dioxide is defined through the pH and the bicarbonate concentration.

The calcite system has the potential to affect the groundwater flow conditions in the rock mass indirectly, due to dissolution and precipitation at different locations in the rock mass. Existing flow paths might be sealed whereas new flow paths might be opened. In addition to the groundwater composition these reactions are also affected by variations in temperature and pressure.

In recharge areas there is, in general, an uppermost layer of the rock where the calcite has been dissolved by the infiltrating groundwater. Such conditions were never observed at Äspö. This would imply that there is no, or very little, recharge of groundwater on the Äspö island.

A large deviation from the equilibrium solubility might indicate errors in analysis or sample treatment. The saturation index (SI = log(solubility/ solubility constant)) is thus a good indicator of sample and analysis quality.

The groundwaters sampled during the pre-investigations were generally slightly supersaturated with respect to calcite. This was thought to be an artefact caused by pumping water from the borehole. Because the drawdown waters from different locations were mixed in proportions different from those of the undisturbed situation and thus the calcite system was not in equilibrium. A similar supersaturation was also expected in the tunnel boreholes and was, as such, included in the predictions. The subsequent evaluation of the tunnel data */Laaksoharju and Skårman, 1995/* shows that the water sampled from tunnel boreholes was supersaturated, as expected, but in some cases also undersaturated. However, there is a general tendency that at deeper sections in the tunnel the calcite system is at equilibrium. A plausible explanation of this is that the groundwater system is more homogeneous and more stable at depth, and that the drawdown caused by the tunnel has not changed the proportions of the different water types in the deep part of the rock, as much as it has changed the conditions at shallower depths.

6.2.6 Redox reactions (processes)

Redox conditions are important for the safety assessment of a nuclear waste repository */SKB, 1995/*. The observed redox potential (Eh) and the redox buffering constituents in the groundwater are extremely sensitive to disturbances caused by sampling and analyses. The redox buffer may ultimately be provided by the fracture filling minerals in contact with the groundwater and by the biological processes */Banwart,ed. 1995/*.

Great efforts were made to investigate and solve the issue of deep groundwater redox conditions */Grenthe et al, 1992/.* The present understanding is that the ferrous and ferric iron minerals generally govern the redox properties. This is also the case for data from the investigations at Äspö. However, occasionally other systems are thought to dominate, e.g. the uranium system */Ahonen et al, 1992/.* Regardless of which system controls the Eh it has been clearly demonstrated that the deep groundwaters are generally reducing.

The redox-sensitive elements, for which analyses are normally made are iron (total and ferrous), manganese, sulphide, uranium and dissolved oxygen. As expected, there are normally no measurable concentrations of dissolved oxygen, but the sensor is needed to register any disturbances in the groundwater pumping and sampling procedure. A zero reading of the dissolved oxygen content indicates that the water is anoxic.

Eh measurements are made using three types of electrode, gold , platinum and glassy carbon. Only the complete chemical characterization (see *Table 6-3*), included the proper Eh measurements in the pre-investigations. The measurements were continued for a period of several days (weeks) until the readings levelled out at roughly the same value for all three electrodes. This is the reported Eh value. During sampling in the tunnel no Eh or dissolved oxygen contents were measured, except for those in the redox experiment */Banwart et al, 1995/.*

The enhanced water flow in the upper part of the rock, caused by the inflow to the tunnel, was expected to transport oxygenated water down into the fracture zones and enter the tunnel. This phenomenon was studied in a fracture zone at a depth of 70 m below ground level */Banwart et al, 1995/.* The predictions of oxygen breakthrough failed because the effects of biological oxygen consumption were not taken into account. The conclusion is that an enhanced groundwater inflow does not cause oxygenated water to reach any greater depths, as long as the amount of organic matter is larger than the amount of dissolved oxygen. These conditions could of course vary from place to place but as a starting point the situation at Äspö could also be expected at any other place. At the Stripa mine, for example, where the hydrology had been affected by the drawdown by the mine gallery for several decades, there was no oxygen in the infiltrating groundwater at a depth of 400 metres. Most evidence suggests that the penetration depth for oxygen is a maximum 100 m for the undisturbed conditions and it is not expected to be significantly deeper under disturbed conditions. The effective oxygen consumption by bacteria strengthens the general opinion that anoxic (oxygen free) conditions could always be expected in the deep groundwater.

The Eh value is coupled to the pH value. An empirical relation is a decrease of 60 mV with an increase of one pH unit. At pH 7 the Eh values are mostly between -100 and -300 mV. Plots of the Eh-pH data from the pre-investigation phase and from a few observations in the tunnel are shown in *Figure 6-13.* At these low Eh-levels uranium exists in a reduced (+IV) form and is extremely insoluble.

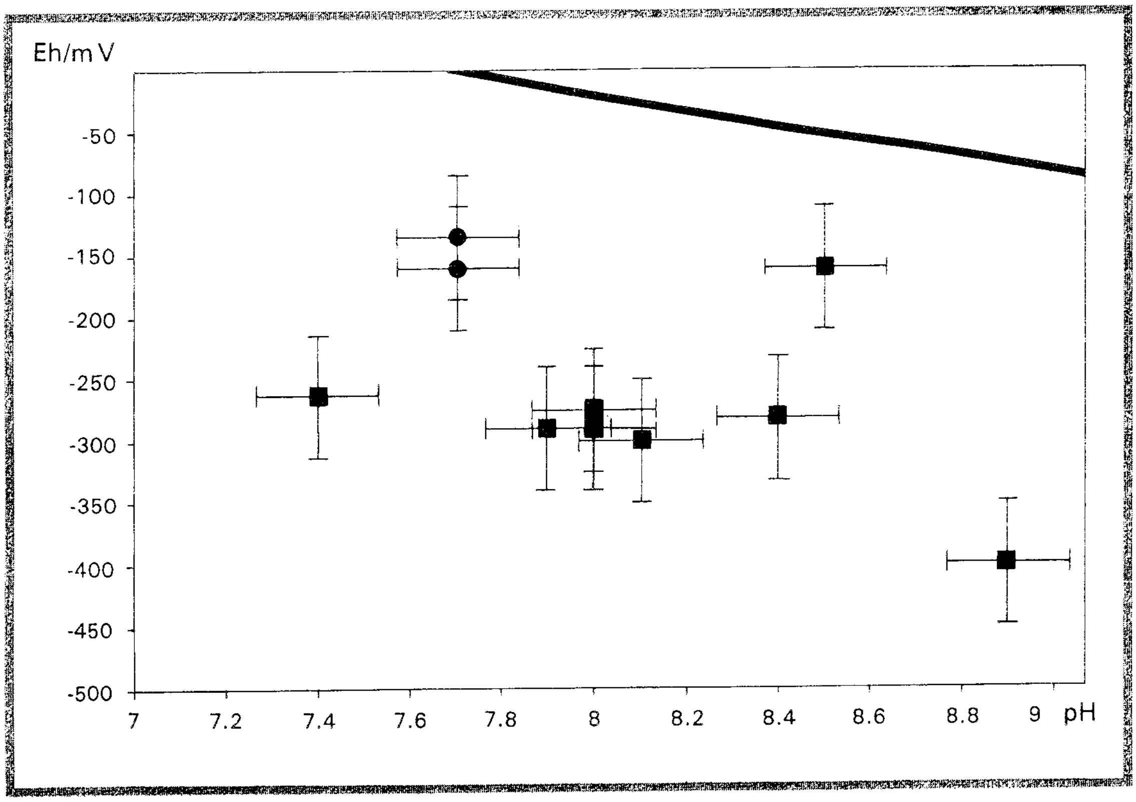


Figure 6-13. *Eh versus pH for the data obtained from the pre-investigation phase (squares) and from the construction phase (Circles). The uncertainty in Eh is estimated to be ±50 mV and the uncertainty in pH is ±0.1 pH unit. The figure includes the calculated Eh for the equilibrium between* UO_2 *and dissolved* UO_2^{2-} *at a concentration of 10 ppb.*

A practical approach for nuclear waste disposal safety assessment is therefore to define reducing conditions to be when uranium (plutonium, technetium and neptunium as well) exists in a reduced form, and oxidising conditions when uranium exists in the hexavalent (+VI) state. The usefulness of this approach is that it resembles well the conditions of the iron system. Under reducing conditions ferrous iron is present in the groundwater in measurable quantities, above ppb levels. In this context it might also be worth mentioning that there is a large difference between reducing and anoxic conditions. Anoxic conditions only mean that there is no measurable amount of dissolved oxygen in the water, whereas reducing means that the Eh value needs to be low enough to have uranium in a reduced form (concentrations at ppb levels). A reducing groundwater is always anoxic.

6.2.7 Biological processes

The microbes themselves do not create new reactions, but they catalyse reactions which would otherwise not take place, e.g. the reduction of sulphate to sulphide and dissolution and reduction of ferric iron minerals. At Äspö the biological processes turned out to be even more important than the chemical interaction between the groundwater and the minerals. The microbial processes always involve redox reactions. They mostly also produce (or consume) carbon dioxide and thus affect both the calcite and redox systems. Because of the unexpected effects of the biological processes the observed bicarbonate, sulphate and iron concentrations were different from those predicted. This was especially noticeable in the tunnel sections passing below the sea, where the water percolating through the seabed sediments transported large quantities of organic matter into the rock. *Figure 6-14* presents the predicted and observed chemistry of the groundwater from fracture zone NE-3. The low sulphate concentration correlates well with the high bicarbonate concentration as a result of the reduction of sulphate and oxidation of organic matter.

The biological processes were not considered to be of importance at the time of prediction, before the tunnel construction was started. But now we know that the bacterial activity has influenced the chemistry and greatly affected both the redox and calcite systems. It has increased the iron concentration up to 4 mg/l and the bicarbonate content up to 800 mg/l, in the fracture zones NE-3 and EW-3.

The observed biological processes are */Pedersen and Karlsson, 1995/*:

- oxygen consumption by oxidation of organic matter
  $O_2 + (CH_2O) \rightarrow CO_2 + H_2O$
- reduction of iron(III) minerals through oxidation of organic matter
  $4Fe(III) + (CH_2O) + H_2O \rightarrow 4Fe^{2+} + 4H^+ + CO_2$
- reduction of sulphate by oxidation of organic matter
  $SO_4^{2-} + 2(CH_2O) + H^+ \rightarrow HS^- + 2H_2O + 2CO_2$

These three reactions will continue until one of the components involved in the process has been depleted. In the Äspö case, aerobic respiration continued until all the dissolved oxygen was consumed */Banwart et al, 1995/*.

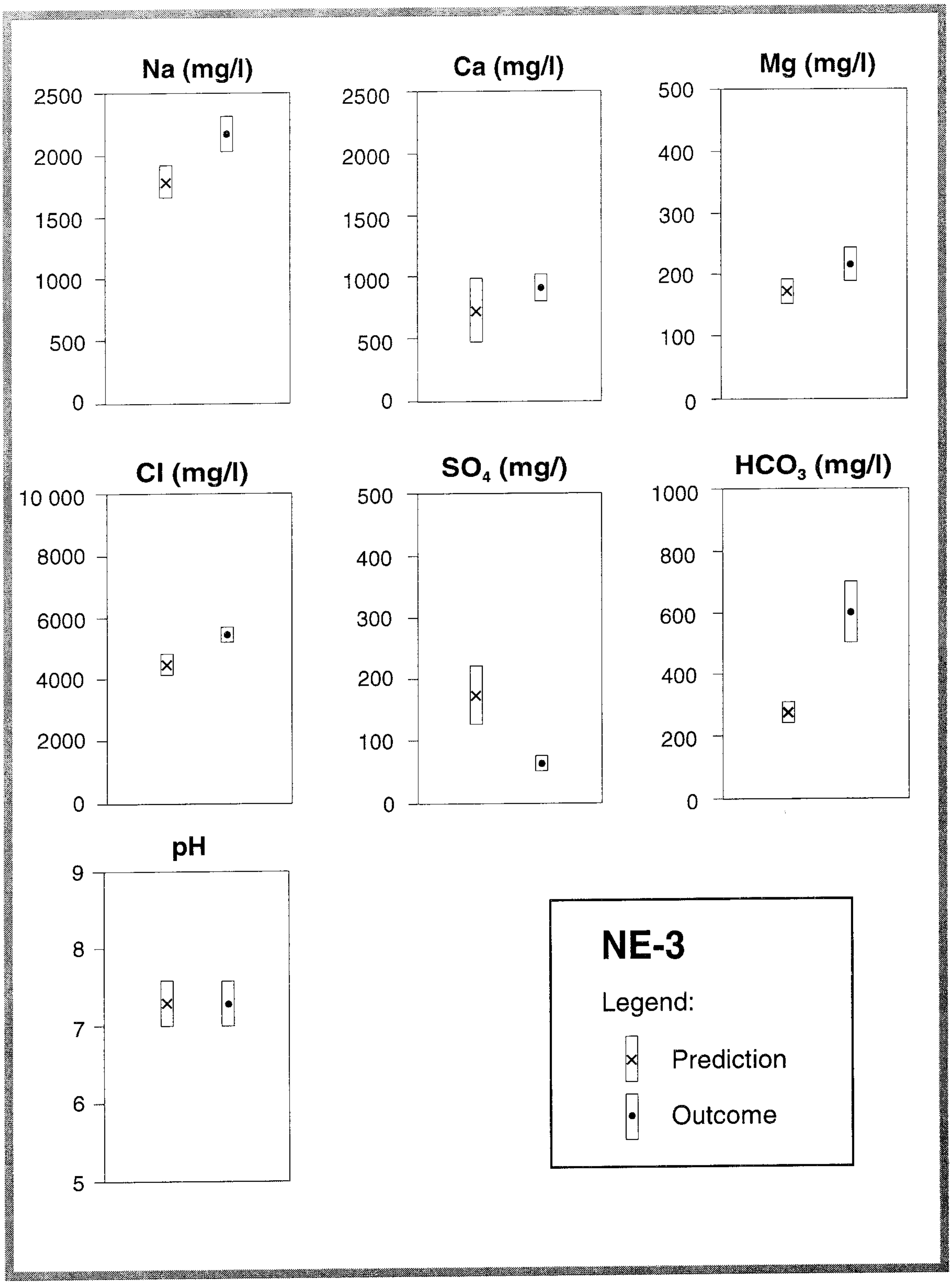


Figure 6-14. Predicted and observed groundwater chemistry of fracture zone NE-3.

The sulphate reduction has been most effective in the tunnel sections where modified seawater containing large quantities of organic matter has infiltrated the rock before and during tunnel construction */Laaksoharju, ed. 1995/.*

6.2.8 Ion exchange

The ion exchange reactions probably affect the ratio of sodium/calcium, especially during episodic events when sea water and glacial melt water are infiltrating into the bedrock. It has been suggested that the calcium in the Äspö redox zone groundwater at 70 m depth could be the result of ion exchange which takes place with the infiltrated old Baltic Sea water */Bruton and Viani, 1994/.* The ion-exchange potential of the site is supported by the occurrence of clay minerals etc.

6.3 GROUNDWATER CHEMISTRY PREDICTIONS

6.3.1 Scope and limitations

Hydrochemical data from the pre-investigations were evaluated by univariate and multivariate analyses. The result of the evaluation was *Model 90* as described briefly in *Section 6.2.3.* It was mainly the water-conducting fracture zones which had been sampled during pre-investigations and therefore also those which were predicted. However, the conditions were also thought to be valid in the intact rock mass where no water samples had been taken. The groundwater composition was extrapolated by linear regression between the observation points.

For the purpose of making detailed predictions it was necessary to focus on the different constituents in the groundwater one by one. The concentration of each constituent was related to the geometrical position (x,y,z) where the sample was collected during the pre-investigations. In the same manner, the predicted values were calculated for the corresponding (x,y,z) where the tunnel was expected to intersect a water-conducting feature. *Figure 6-15* illustrates the position of the data used for the predictions and the position of the observations along the tunnel.

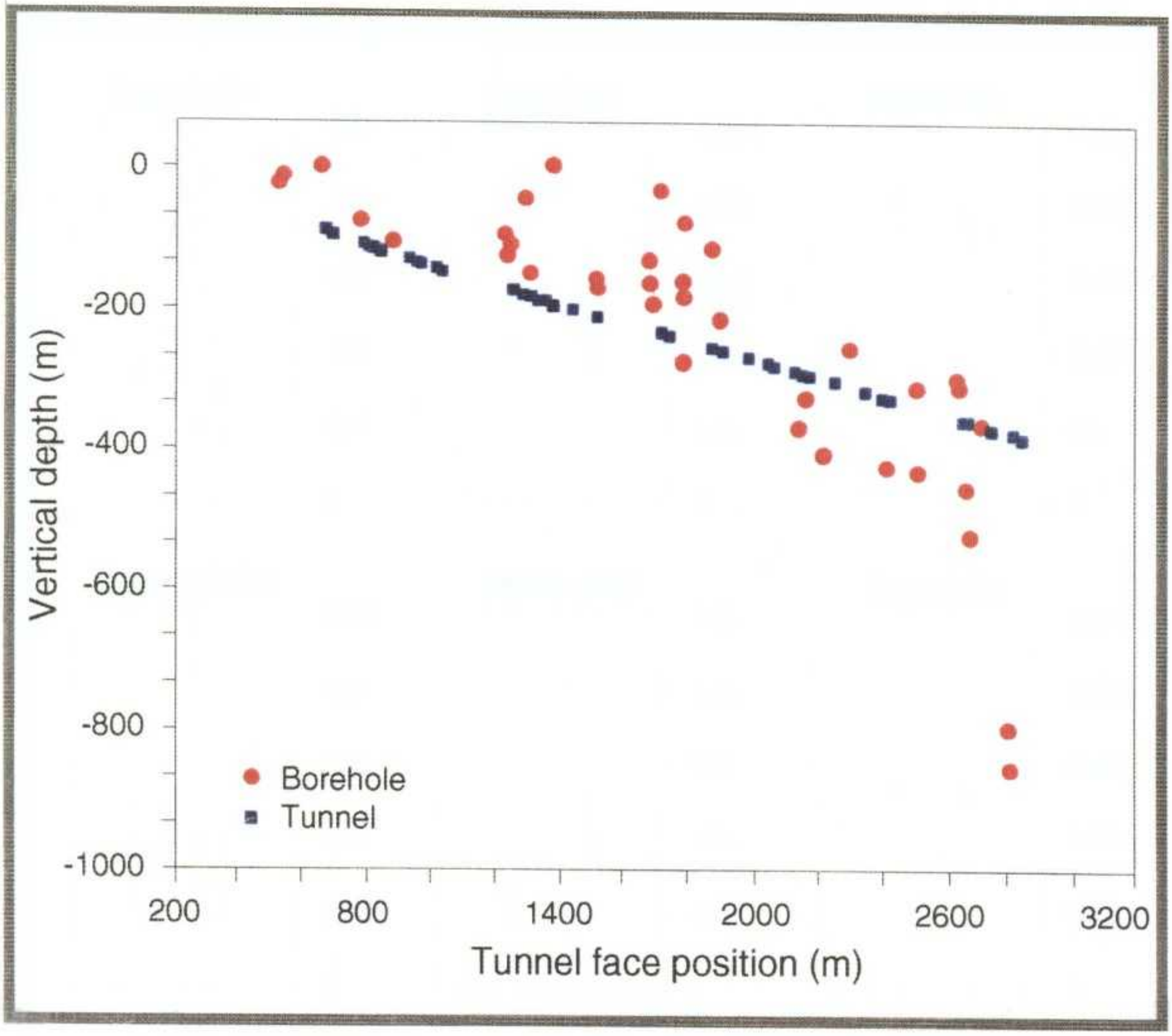


Figure 6-15. *A schematic illustration of the position where the data were collected for the hydrochemical predictions and where in the tunnel the observations were made for comparison with the predictions. It should be mentioned that all the positions of the pre-investigation boreholes are not in the plane of the tunnel. Vertical section according to A-A' in Figure 2-6.*

An important limitation in this approach was the necessity to consider the hydrochemical system in a steady state, where the conditions observed during pre-investigations would remain unchanged during the tunnel construction. Of course this was not entirely expected to be the case, but the reason for making this assumption was that there were no established methods that could be used to make a transient hydrochemistry model for the tunnel excavation phase. The first sample collected immediately after drilling of the probe holes in the tunnel front was thought to be a good reference of undisturbed conditions. Thus assumed that only minor disturbances would have taken place before sampling, giving that the comparison with the predicted situation would be correct. This is illustrated by the predicted and observed element concentrations in groundwater from fracture zone NE-1 (*see Figure 6-16*). The approach of

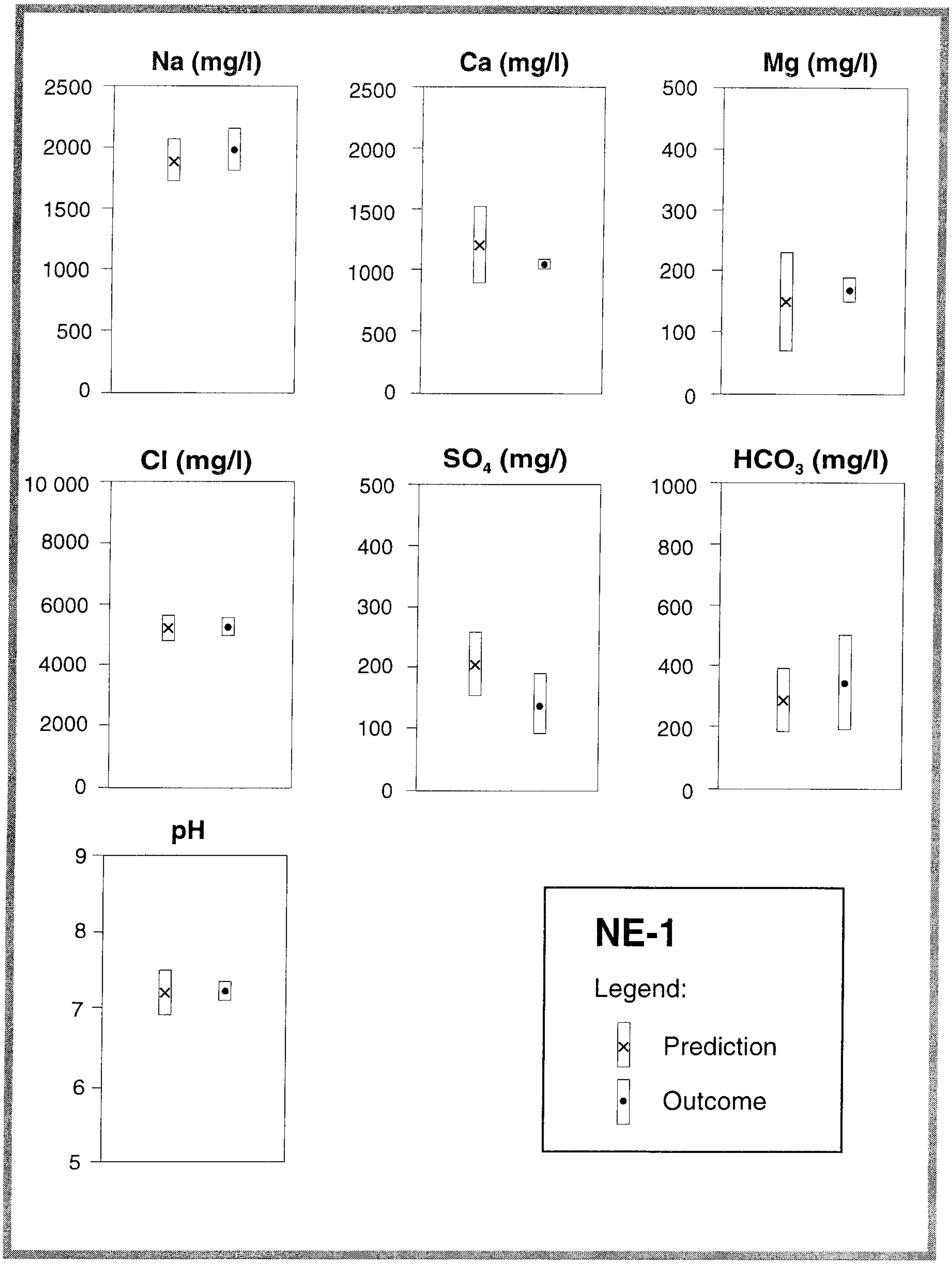


Figure 6-16. *Predicted and observed element concentrations in NE-1.*

finding the undisturbed conditions in the tunnel front was expected to be correct through the straight part and the first turn in the spiral. However, the information in *Figure 6-14* (earlier presented), with prediction and observations in NE-3, does not reflect as good agreement as for NE-1. The reason for this is probably the difference in the amount of data available from the pre-investigations. NE-1 was chemically sampled from three boreholes while NE-3 chemistry was evaluated from one single sample of one borehole.

The concentrations of major constituents were predicted for every tunnel position where a discrete water-conducting feature was expected to intersect the tunnel. *Report 4* of this series */Rhén et al, 1997b/* contains a systematic comparison of all the predictions and outcomes. *Figure 6-16* shows the comparison between prediction and outcome for NE-1. In this case all the predicted and observed concentrations agree. *Figure 6-14* shows the corresponding predictions and observations for NE-3. In this case only the pH, calcium- and magnesium concentrations agree whereas, for example, the predicted concentrations of sodium, chloride, sulphate and bicarbonate disagree (cf. *Section 6.3.2* for discussion).

Transient predictions were also made. In some major conductive zones and five selected borehole sections the chemical composition and transport of solutes were predicted for undisturbed conditions before starting the excavation of the HRL tunnel and for successive intervals as the tunnel approached its final length */Rhén (ed), 1991, Gustafson et al, 1991/*. *Table 6-4* shows the predicted groundwater chemical composition of fracture zones NE-1, NE-2 and NNW at their intersection with the tunnel.

The predictions were based on the knowledge gained during the pre-investigation programme about natural chemical conditions before the start of tunnel excavation, i.e. groundwater samples in borehole sections. The chemical data were then related to the structural model of the Äspö island, including fracture zone geometry, interconnections, hydraulic conductivity, porosity and measurements of natural flow rates, hydraulic heads and estimated flow directions.

In the prediction of the disturbed conditions four chemical end-members were considered 1. Rainwater, 2. Shallow groundwater, 3. Baltic seawater and 4. Fracture-zone groundwater. The last one, fracture-zone groundwater, is specific to every fracture zone and varies depending on which fracture zone is considered and also the depth in the zone. The predictive calculations were mainly made utilizing simple analytical expressions, but also principal component analyses were used.

The combined effect of sparse predictions (with only a few points in tunnel and surface boreholes with complete time series of chemical, head and flow data) together with changed tunnel lay-out, revised fracture zones and changed chemical end-members makes evaluation of prediction reliability cumbersome. However, the overall conclusion is that the predictions made during the pre-investigation as a whole are in accordance with the outcome, although the tunnel breach of zone NE-1 changed the flow and chemical composition in zones NE-2 and NNW-4 to a larger extent than was predicted. The surface type of waters also penetrated the fracture zones to a lesser extent than expected from the predictions.

Table 6-4 presents the fracture zone groundwaters predicted to be found in specific tunnel situations during excavation.

Table 6-4. Prediction of groundwater chemical composition at the location of the HRL tunnel intersection with fracture zones NE-1, NE-2 and NNW at successive intervals (Tunnel Face Position, TFP) during the tunnel excavation. Compiled from */Gustafson et al, 1991/.*

Conductive zones	TFP m	Na mg/l	K mg/l	Ca mg/l	Mg mg/l	Cl mg/l	HCO_3 mg/l	SO_4 mg/l	Fe^{tot} mg/l	pH	Eh mV
NE-1	700-1475	1900 ±200	31 ±20	1200 ±350	150 ±80	5300 ±400	290 ±100	210 ±50	0.6 ±0.6	7.2 ±0.3	-230 ±25
NE-1	3064-3854	2000 ±500	8 ±5	2000 ±800	80 ±20	7000 ±2000	14 ±5	320 ±80	0.3 ±0.3	8.0 ±0.5	-340 ±25
NE-2	1475-2265	1200 ±300	5 ±5	1100 ±300	30 ±30	3800 ±1000	70 ±50	140 ±40	0.3 ±0.3	7.7 ±0.1	-290 ±25
NNW	1475-2265	500 ±200	5 ±5	400 ±200	30 ±300	1500 ±1000	150 ±50	150 ±50	0.3 ±0.3	7.8 ±0.2	-300 ±25
NNW	2265-3064	800 ±300	7 ±5	800 ±300	40 ±30	2500 ±1000	170 ±70	120 ±80	0.3 ±0.3	7.7 ±0.3	-290 ±25
NNW	3064-3854	1000 ±500	8 ±5	1000 ±500	50 ±20	3500 ±1000	120 ±20	160 ±80	0.3 ±0.3	7.6 ±0.2	-290 ±25

6.3.2 Spatial assignment methods

Initially (before tunnel construction was started) the predictions were made by a combination of principal component analysis and expert judgement. The predicted values were fairly easy to calculate, but the variability had to be estimated. At an early stage of the tunnel construction phase, it was evident that there were many disagreements between predictions and observations. It was not clear why there were large discrepancies, because sometimes, in the case of NE-1, for example, there was agreement between predictions and observations. However, one explanation could be that an unsuitable method had been used for the predictions. Therefore, tests of different interpolation methods were made to see which could be used to perform spatial assignment of groundwater chemistry properties. The tested tools were:

- Linear regression analysis
- Principal component analysis
- Kriging
- Neural networks

The multiple *Linear regression* model is based on the least-square method. The linear regression analysis minimizes the distance between the observations and a straight line as a function of the position (x,y,z). The basic requirements of the model are that the observations be independent, normally distributed and have the same variance. In order to give a good correlation all observations need to be linearly dependent on the position (x,y,z). The computer program used was *STATISTICA for Windows /1994/* and *STATGRAPHICS PLUS for Windows /1994/.* Separate calculations were made for each of the major components separately.

Multivariate (principal component) analysis is a mathematical way of treating the different parameters all together. The values to be predicted could be considered as missing data in a matrix. The principal components are computed directly from the known data values as a linear function of all the underlying parameters. The principal components are independent and extrapolated to the position (x,y,z). A predicted value for each constituent is recalculated from the linear correlation of the principal component as a function of position. The method used was *Fillas* in the computer program PARVUS */Forina et al, 1988/.*

Kriging is an interpolation method based on a non-linear correlation function. The basic assumption is that the modelled properties are continuous and that positions physically close to each other also have properties numerically close to each other. Thus, an observation physically close to a position to be predicted has a larger weight than an observation which is physically further away from the position to be predicted. The correlation function is obtained from the calibration data and the predictions are more uncertain the further they are from an observation. All values have an uncertainty, a variance, associated with them. There are different ways of estimating the unknown values and their corresponding variances. The computer program used was *SURFER for Windows /1994/.* Separate calculations are made for each element to be predicted.

Neural networks contain artificial neurones organized in layers and connected to each other in a way simulating the human brain. Each neurone in a layer is connected to all neurones in the previous and the following layers. The connections between the neurones have different strengths. The neurone computes its output signal as a weighted sum of its input signals. Neural networks learn by associations, from examples, by comparison, and by repetition. The neural network is non-linear, highly interconnected and is therefore able of capturing complex relationships between input and output. Thus, neural networks possess an ability to treat complicated non-linear problems, generalize, analyse large amounts of data, interpolate and optimize data. The software *BRAINMAKER PROFESSIONAL for Windows /1993/* was used to create, train and run neural networks */Hecht-Nielsen, 1991, Hertz et al, 1991 and Lawrence, 1992/* on the chemical data in both the pre-investigation and construction phases.

Only principal component analysis was performed in the phase of initial predictions. The same data set - the pre-investigation data - was later used to make 'predictions' using the other methods as well. The careful testing of the different tools shows that there are differences in the results which could be related to a systematic difference in the way they are constructed. Some general conclusions are:

- The principal component analyses and linear regression analyses give a larger difference between predicted and observed concentrations than the other two methods. This is probably due to the fact that these methods only include linear combinations, in this case the predicted value as a linear function of the data from co-ordinates (x,y,z).

- Neural networks and kriging reflect surprisingly well the trend in the variations in the concentrations and are therefore also closer to the observations. Kriging is generally closer than the neural network but the differences are small.

Figure 6-17 illustrates the predicted and observed chloride concentrations along the tunnel for all the tested methods.

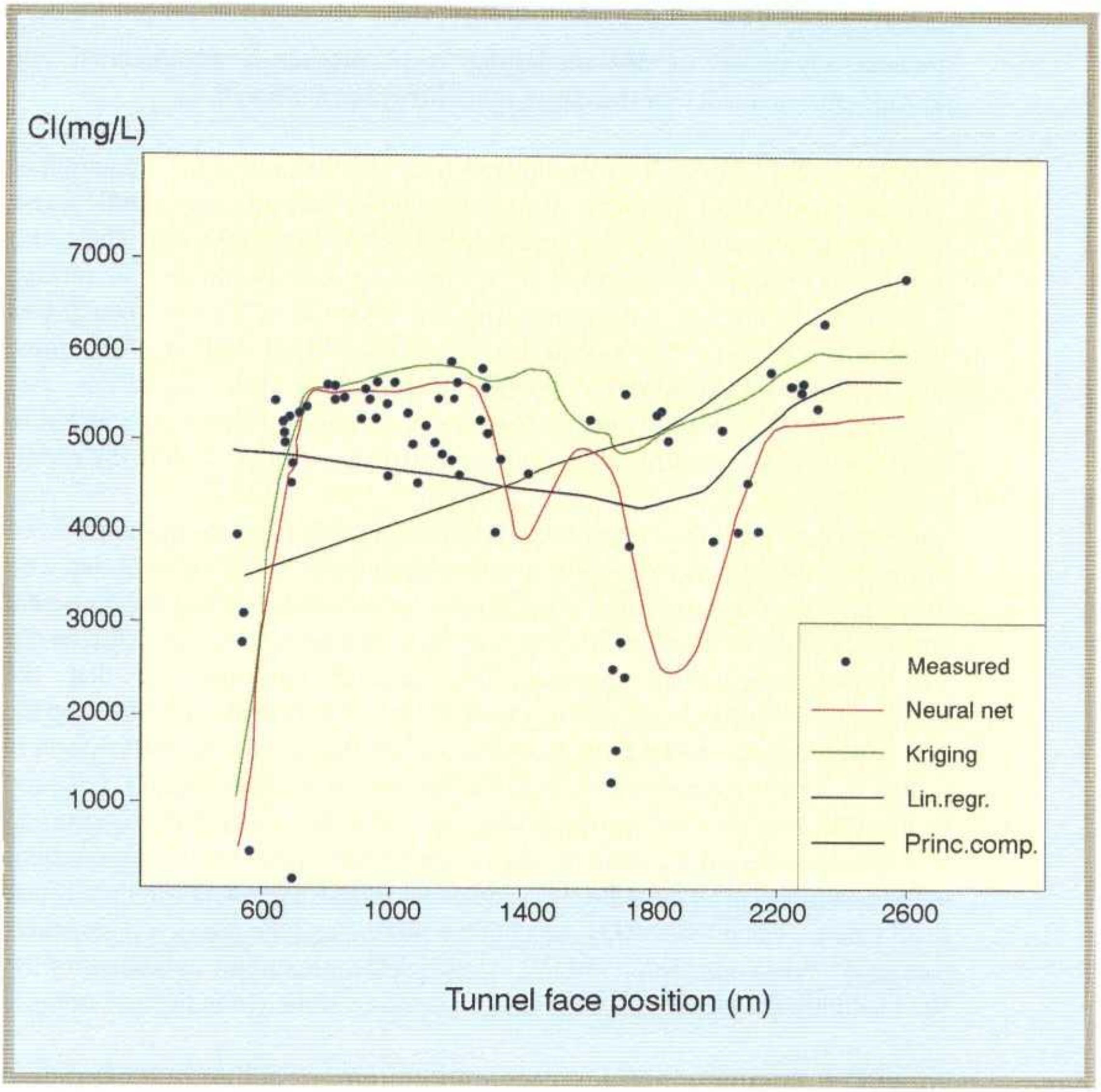


Figure 6-17. Predicted and observed concentrations of chloride calculated by different mathematical methods, but with exactly the same input data.

6.4 EVALUATION OF MATHEMATICAL TOOLS

6.4.1 General

Hydrochemical evaluation has traditionally been a "handicraft" for specialists, but in addition to that there are now several different computer codes available which improve and simplify evaluation and interpretation. This work has made extensive use of the *M3* modelling concept, see *Section 6.4.2. M3* stands for Multivariate-Mixing and Mass balance calculations. The program package was developed during the course of the Äspö project. It includes principal component analyses designed to identify end-members and define reference waters for mixing calculations. The mass balance calculations are then used to calculate how much of the variables cannot be accounted for by mixing. The greatest advantage of *M3* modelling is to provide a documented and reproducible sequence of the entire modelling, see *Section 6.4.2*.

There are other numerical codes which can handle both mixing and reaction as well as transport and reaction. These computer codes can only handle a few reactions which are pre-set or a few free variables simultaneously. The codes mostly assume that the reaction is the dominating process and that the mixing is a secondary process. An example of such a code is NETPATH which was also frequently used for evaluating Äspö data. PHREEQE was the most commonly used equilibrium reaction code in the data evaluation. The calculations were used to check the status of reactions which are expected to be at equilibrium, mainly calcite, but also other fast reactions were checked.

The improvement of the evaluation and prediction methods by using standardized mathematical/statistical tools has two major advantages. The first one is that with the computer-based programs it is much easier to assess and control and document the quality of the evaluation and the prediction procedures compared with the use of 'expert judgement' methods. The second advantage is that the mathematical/statistical methods are reproducible and not entirely dependent on the person who does the modelling. A general way of adapting the modelling tools is to start by expert methods, to 'look at the data and try to understand it', followed by a thorough multivariate (principal component) analysis. After the PCA the end members involved in the groundwater should be identified and the proportion of the end members in all the collected samples calculated. The integrated mixing and mass balance calculation *(M3)* sorts out the mixing and the reaction proportions (see *Laaksoharju and Wallin /1997/*). A good description of the conditions of the site facilitates the prediction of the future evolution of the groundwater system.

An attempt was made to achieve more sophisticated modelling of the transient situation during tunnel construction. The inflow to the tunnel was used to calculate the water flow in the different fracture zones intersected by the surface boreholes. Using the calculated flow in the packed off monitoring sections and the assumed flow porosity of the water conductors it was possible to calculate the groundwater volumes transported through the rock volume. It was also possible to calculate the way in which the different water types were transported through the different fracture zones. For a more detailed and comprehensive prediction of this type, it would be necessary to develop a computer code. The manual calculations are time consuming. For these mixing calculations only three water types were used, deep saline water, sea water and meteoric freshwater. A detailed discussion on these 'predictions' is given in */Ittner and Gustafsson, 1995/* and is briefly described in */Rhén et al, 1997a/*.

6.4.2 Multivariate Mixing and Mass balance calculations *(M3)*

The origin and evolution of the groundwater can be described if the effect from mixing and reactions can be examined separately. In order to do this separation a new method named Multivariate Mixing and Mass balance calculations (abbreviated to *M3*) was constructed. The model consists of 3 steps where the first step is a standard principal component analysis, followed by mixing and finally by mass balance calculations.

The M3 calculations contain the following steps:

1. A standard multivariate technique, called Principal Component Analysis (PCA) is used for cluster analyses of the data by using the major components Cl, Ca, Na, Mg, K, SO_4 and HCO_3 in combination with the isotopes δD, $\delta^{18}O$ and ^3H. The PCA aims to describe as much of the information from the ten variables in the first equation called the first principal component as possible. The rest of the information is described by the second principal component and so on. The Principal Components are calculated as linear combinations of all variables in a way to minimize the difference (error) between the model and the data. The components are derived in decreasing order of importance. Generally the first Principal Components will account for most of the variation in the original data.

   The first principal component is applied to the initial data. The variation not accounted for by the first principal component is described by the second principal component and so on. For the Äspö hydrochemistry data the first three principal components were calculated and analysed. It turned out that the first two components did describe the system well enough, whereas the third component mainly described the disturbance caused by drilling and pumping in one single deep borehole at Laxemar, KLX02, see */Rhén et al, 1997b/.* For the first two principal components an x, y scatter plot can be drawn. The x is the equation for the first principal component and y the equation for the second principal component. The plot is named the *M3 plot* and is used to visualise the clustering of the data as well as to identify extreme waters. Extreme waters are called *end-members* or *reference waters*. A reference water is a well-sampled groundwater which resembles an assumed or modelled end-member eg. Glacial meltwater (see *Figure 6-18a* and *b*) Lines are drawn between the reference waters so a polygon is formed. By definition the selected reference waters can describe the observations inside the polygon. The observations inside the polygon are compared to the chosen reference water compositions.

2. Mixing calculations are used to calculate the mixing portions of the reference waters or the end-members. The mixing portions describes the different reference waters in the observed water. The calculated mixing portion can be used to evaluate the origin of the groundwater. The mixing portions are equal to the trigonometrical distance to the selected reference waters or end-members in the *M3 plot* (see *Figure 6-18c*).

3. Mass balance calculations are used to define the sources and sinks for different elements which deviate from the ideal mixing model used in the calculations *(see Figure 6-18d).* The mixing portions together with the composition of the reference waters are used to calculate new values for

each point. No deviation between the measured and calculated value indicates that mixing can explain the element behaviour. A source or sink is due to reactions. The evolution of the groundwater can thus be described.

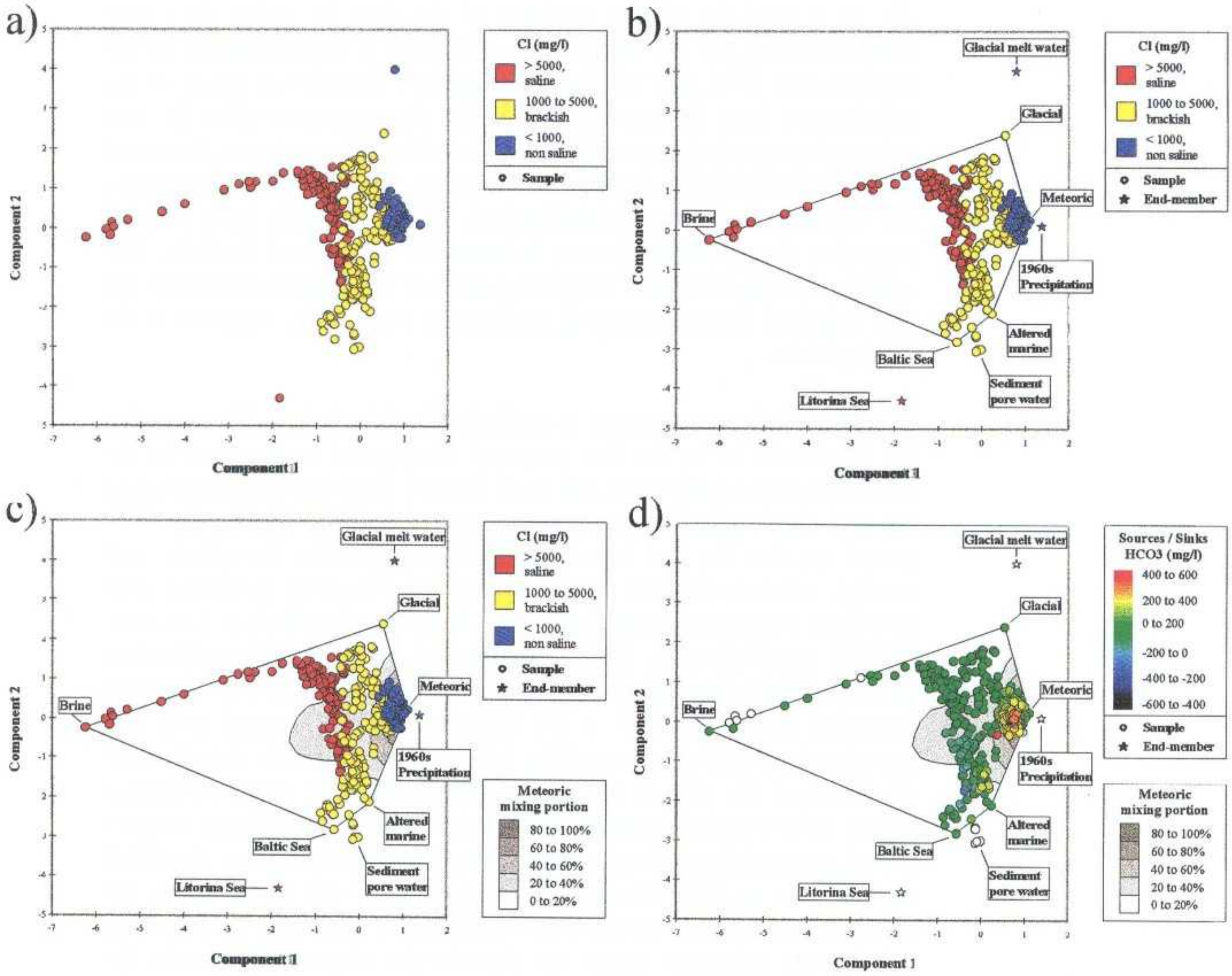


Figure 6-18. *Different steps in the M3 modelling; a) principal component analysis is used to obtain the maximum resolution of the data set, b) selection of end-members and reference waters - the other groundwaters are compared to these, c) mixing calculations - portions of meteoric water are shown in the figure, d) mass balance calculations - the sources and sinks of eg. Carbonate are shown which cannot be accounted for by mixing. The groundwater samples in Figure a, b and c have been colour coded based on the Cl-content into saline, brackish and non-saline groundwater.*

The *M3* model can describe the groundwater chemistry as a result of mixing and mass balance reactions. It is important to note that the modelling is always relative to the selected reference waters or end-members. The boundary conditions of the modelling can be changed depending on the selection of reference waters or end-members. A calculated portion of e.g. Glacial water based on the reference water composition may be 50% higher than when the calculation is based on an end-member composition.

The advantage of using a reference water rather than an end-member is that the composition of the end-member is never as well known as for the reference water. Effects of reactions can therefore only be revealed for calculations that are based on reference waters.

6.5 EVALUATION OF SITE INVESTIGATION METHODS

Groundwater chemical properties were investigated by sampling in boreholes on different occasions. *Figure 6-1* illustrates the different sampling methods and the evaluation of the data.

Most important for defining the chemical composition of the groundwater in major fracture zones was the chemical characterization of the groundwater by using a mobile field laboratory with the downhole measuring devices, *CCC* in *Table 6-2*. The second most useful method was the sampling along with the interference pumping tests, *SPT*. A third useful method was the sampling in percussion boreholes, *3P*. Due to contamination the samples collected during drilling *SDD* were not useful.

Lightweight portable sampling equipment was developed for sampling in percussion boreholes. The equipment consists of a packer, a pump and tubes and is operated by a gas pressure, *3P*. This unit was most useful for the very first sampling of percussion boreholes when there were no roads to the boreholes.

The sampling during drilling of the deep cored boreholes was not useful since the water was always highly contaminated by drilling water. Nevertheless, these data were used to describe the groundwater composition in those fracture zones where no other kind of sampling was performed. In many cases the content of drilling water was up to 50% or more.

The results of the flow-meter and spinner survey were successfully used to select the borehole sections for the complete chemical characterization, and for interference pumping tests. A combination of different geophysical logs cannot provide the same exact identification of the hydraulic sections in the hole. However, a good overall picture of transmissive borehole sections was obtained by combining fracture frequency, single point resistance and sonic logs */Smellie and Laaksoharju 1992/*.

The combination of complete chemical characterization (*CCC*) and sampling during pumping tests (*SPT*) is very favourable, since *SPT* is a much faster procedure and can thus be conducted at a large number of borehole sections in a relatively short time. A further advantage of the *SPT* is the fact that the results of the hydraulic interference test can be used in the evaluation of the hydrochemical results. Due to the large volumes of water pumped out it is possible to evaluate the chemical transients and thus be able to trace the flow direction.

The poor usefulness of sampling during drilling (*SDD*) was due the fact that the sample often contained up to 50% of drilling water. Methods to avoid the contamination of samples by large quantities of drilling water, has been in focus during the drilling at Äspö, where the so-called telescope type drilling technique[1] was used. The advantage over ordinary core drilling, is that more water is pumped out of the borehole than is pumped down as drilling water. This procedure was not sufficient to provide representative samples during drilling. Further improvement of the drilling technique and an improved sampling technique is needed, and has now been made.

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.

There are different needs for hydrochemical data. These can be grouped into three categories:

- Reliable data on safety related parameters such as pH, Eh, redox and pH-sensitive 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, a well-defined classification of information levels can be achieved:

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[1] The telescope type drilling technique involves ordinary core drilling to 100 m. Before the drilling is continued the hole is reamed to a diameter of 110 mm, making it possible to pump out the water as the drilling is continued.

i Major constituents, sodium, potassium, calcium, magnesium, bicarbonate, chloride and sulphate are unaffected by disturbances from drilling or contamination from other investigation methods, as long as the proportion of drilling or testing water can be analysed, and corrected for.

ii Trace elements and stable oxygen-18 and deuterium isotopes are reliable even with a content of up to 5% of drill flushing water.

iii pH-sensitive trace elements, tritium and carbon-14 data are reliable only when the contamination by drilling water or meteoric water entering through the borehole is less than 0.1%.

iv Eh and redox-sensitive elements are reliable when the electrode readings have stabilized and the Eh value can be interpreted. Normally several days of continuous pumping is needed with measurements in on-line flow through cells, and preferably downhole measurements of Eh and pH.

With the techniques used at Äspö, *Level iv* can only be reached using the procedures for complete chemical characterization, *CCC*. An improvement in the procedures and technique of sampling during interference pumping tests could perhaps result in *Level iv* data.

Level iii is reached by the *CCC* and the pumping tests, *SPT*. A modification of the pumping technique, which has now been made, makes it possible to achieve reliable pH readings as well for *SPT*. Reliable Eh data would need much longer pumping time.

Sampling during drilling and sampling with the *3P* equipment provided data of *Level I*. A more carefully planned drilling and sampling procedure should give data of *Level ii*. A more comprehensive development of down-hole samplers could perhaps result in data of *Level iii*. This possibility is now being tested.

A subjective judgement of the usefulness of the sampling procedures is given in *Table 6-5*.

Table 6-5. Judgement of usefulness of different investigation methods from the pre-investigation phase of the Äspö HRL.

Subject	Methods		Usefulness	
		Block scale	Detailed scale	Site scale
Groundwater chemistry in major fracture zones	Sampling in percussion-drilled holes			
	-3P	2	-	-
	Sampling in cored holes			
	-SDD	1	-	-
	-SPT	2	-	
	-CCC	3	-	
	Clean-out pumping	1	-	
	Spinner survey	2*	-	-
Quality changes and redox conditions	Sampling			
	-CCC	-	2	-
	-SDP	-	1	-

Very useful = 3 Useful = 2 Less useful = 1 Not applicable = -

* Not used as a single method

6.6 OVERALL EVALUATION

6.6.1 General

A hydrochemical model is the description of the groundwater chemistry and the processes responsible for the observed chemical composition. By careful investigations it is possible to obtain a good picture of the present chemical conditions of the groundwater. The pre-investigations at Äspö aimed at giving a good enough description, for the performance assessment of a nuclear waste repository site of the variability of the groundwater chemistry and the most important processes affecting the groundwater composition. These are:

- Mixing of water from different origin.
- Biological processes which are mainly affecting the conditions below the sea bottom.
- Chemical reactions mainly calcite equilibration and long-term water-rock interaction.

From a hydrochemical point of view, the conditions at Äspö were optimal for evaluating the processes behind the observed groundwater chemistry. The increase in salinity with depth gave a possibility to differentiate between the effects of mixing and the effects of groundwater/rock interaction. This led to the conclusion that mixing is more important than groundwater/rock reactions for the chemical composition. The results indicate that mixing has been concentrated to episodes in the period lasting from the last glaciation up to now. Conditions prevailing before and during the glaciation can not be evaluated at present.

With the increased understanding of the processes taking place in the past there is now a good basis for predicting future conditions. *Table 8-1* gives a condensed overview of the important processes and their status after completion of the pre-investigation and construction phase investigations at Äspö.

In a future repository site investigation it is necessary to collect data for two purposes. The first one is to assess the conceptual model of the site. This model is largely expected to be similar to the Äspö site model: The groundwater in the deeper parts of the rock are expected to be more immobile and more affected by water rock interaction than the more shallow parts where mixing of different type of groundwater is more important than the chemical reactions. The second purpose is to obtain the data necessary for describing the processes responsible for the observed groundwater chemistry. In practice there will be no major difference in the way in which the future site investigations will be performed compared to how the Äspö investigations were performed. The main difference will be in the planning and evaluation of the investigations.

Hydrochemical processes

The role and scope of groundwater chemical investigations and hydrochemical modelling of a repository site are to:

- verify the generally known and expected conditions (conceptual model).
- perform tests to show if unfavourable conditions exist.
- provide the input data for site-specific assessment calculations.
- examine the data for unexpected processes which might be of importance for the future evolution of the groundwater chemistry.

The groundwater mixing process has been identified as the most important for the groundwater chemistry. This needs to be checked at a repository site.

The calcite dissolution-precipitation is well established and will eventually control the pH of the groundwater. Data for the calcite system is needed for the calculations.

Redox conditions are expected to be reducing. Initial careful measurements (down hole) are needed to verify this and to ensure that oxidizing conditions do not occur. Data on redox buffers are needed for safety assessment calculations. Biological activity is also affecting the redox conditions.

6.6.2 Models

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. This knowledge is then useful for defining the gradual evolution in the future.

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. 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. Regardless of which, we see the effect as a peak in glacial reference water in fracture zone NE-2 (see *Table 6-3).* 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. On-going work will lead to even better understanding of the biological processes and the possibility of using the model in a predictive mode.

6.6.3 Prediction-outcome approach

There are simple ways of checking the predictive ability of a model. The simplest is to compare the prediction and the outcome to see if they agree. In practice this was the intention when the predictions of construction phase groundwater chemistry were made on the basis of the pre-investigation models. Some general comments on this approach are:

- The initial predictions were based on a combination of expert judgements and principal component analyses. However, the range was only estimated by expert judgements. It seems now that the estimated ranges were too narrow, because the estimate did not include the natural variability, only the uncertainty in the data.

- When the different mathematical methods described in *Section 6.4*, were tested, the range of variation was calculated on the basis of the variation in input data. The same variation was expected for the observations. The result is that most of the observations fall within the predicted ranges for all constituents except sulphate and bicarbonate. In some cases the range of variations is so wide that it could be questioned whether the prediction is meaningful or not. Sulphate and bicarbonate predictions failed in positions where sulphate reducing bacteria have been active.

The approaches to consider the hydrochemistry as a static system reflecting the conditions of the pre-investigations are of course dubious. However, by selecting a suitable predictive tool, kriging or neural networks, the observations all fall within the predicted ranges. It is therefore possible to predict a repository rock volume on the basis of pre-investigation data. Observations must then be made in a way to be comparable to predictions.

The approach of predicting the groundwater composition to be observed during construction might not be worthwhile for a real repository anyway. The reason is that too many conditions which will affect the outcome cannot be foreseen. Also the need for predictions is not urgent, since the chemical conditions during construction are expected to be different from the conditions prevailing after closure of the repository. These conditions are important and probably more close to the initial undisturbed conditions. Therefore, it is important to obtain a good description of the chemical conditions during the pre-investigations when the groundwater system has not been mixed up by drawdown into excavated tunnels. A carefully planned and performed site investigation programme can fulfill such criteria.

Quantitative predictions of groundwater composition are sometimes useful for planning construction work. The salinity of the groundwater has a severe impact on the corrosion of steel constructions in the tunnel. Such predictions could however, be made as quantitative estimates of the salinity, for instance.

If hydrochemical predictions were to be made at Äspö, or elsewhere, they would be based on the concept of mixing and include the mixing proportions of the identified and selected end-members and reference waters. These predictions would have two different purposes. One to assess the long term performance issues and the second to assess the groundwater flow model with the mixing caused by the tunnel draw-down.

6.6.4 New knowledge from the tunnel

The large number of sampling points in the tunnel has given a more detailed picture of the variability of the groundwater chemistry. It has been extremely useful to compare the results from the tunnel section passing below the sea with the results from the tunnel spiral under Äspö. The massive biological activity is concentrated to spots in the tunnel section located below the sea. The sea-bed sediments are likely to feed the bacteria with organic matter.

As important as the large number of sampling points, and time series data from these points, is probably extra given time used for renewed interpretation of the previous and new data together. This has given a more mature model of the hydrochemistry.

6.6.5 Conclusions

- 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. Methods and models have been developed for identifying the different sources of groundwater at the Äspö site and the way in which groundwater at specific locations in the rock mass can be described as a mixture of water from these sources.

- 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. In addition to the inorganic reactions between oxygen and minerals, the effective oxygen consumption by bacteria strengthens the general opinion that anoxic (oxygen free) conditions could always be expected in the deep groundwater, also during the operational phase of a deep repository.

- The observed biological processes are:

  - oxygen consumption by oxidation of organic matter
  - reduction of iron (III) minerals through oxidation of organic matter
  - reduction of sulphate by oxidation of organic matter

- 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 downhole Eh and pH measuring devices. The second most useful method is the sampling during the hydraulic interference pumping tests. A third useful method is the sampling in percussion boreholes. The sampling during drilling was not useful due to uncertainty in the quality and representativity of the water. However, the method for sampling during drilling can be improved so that useful data on the groundwater origin and distribution can be obtained.

- The experiences and knowledge have made it possible to define four practical and relevant levels of chemical information:

  i major dissolved components
  ii i + trace elements and stable isotopes
  iii ii + pH sensitive elements, tritium and carbon-14
  iv iii + Eh and redox sensitive components

7 EVALUATION OF MODELS FOR TRANSPORT OF SOLUTES

7.1 INTRODUCTION

Modelling of the transport of solutes was mainly aimed at describing the salinity distribution in the rock mass under natural conditions and during construction of the tunnel. Predictions were made using the PHOENICS numerical code */Spalding, 1981/* to test its ability to predict the salinity of the flow into the tunnel and in borehole sections. Scoping calculations of flow paths and flow times were also performed to some extent.

The transport-of-solutes model is linked to the groundwater flow model presented in *Chapter 5* as the same geometrical framework is used and the pressure head is dependent on the water density. In the Äspö case it is the salinity of the water that affects the density. In the transport-of-solutes model a few concepts concerning the material properties were added to the coupled model (see *Table 7-1).* The transport-of-solutes concepts are presented in detail in *Rhén et al /1997b/* together with the transport-of-solutes model of Äspö. Concepts for the groundwater flow model are presented in *Chapter 5.* The concepts described in *Table 7-1* formed the base for the numerical groundwater flow modelling of transport of solutes with the PHOENICS finite volume code.

Up to 1995 only a few tests had been made at the Äspö HRL to estimate the transport properties of the rock mass. *Rhén et al /1997b/* contains a brief presentation of these results together with some data from other sites compiled in *Andersson /1995/* in order to give possible values or ranges for some of the transport parameters. The projects at Äspö related to the transport of solutes are briefly presented below. Estimation of the transport properties of the rock mass will be one of the main objectives of future work at the Äspö HRL.

Table 7-1. Condensed description of the transport-of-solutes model of the Äspö site used within the Äspö HRL Project.

TRANSPORT OF SOLUTES MODEL OF THE ÄSPÖ SITE

Scope
Flow paths during natural flow, interference tests and flow to the laboratory tunnel.
Solute transport of non-sorbing elements.
Solute transport of elements affected by retardation.

Process description
Flow processes - see process description for groundwater flow.
Advection.
Hydrodynamic dispersion (mechanical dispersion + molecular diffusion).
Retardation (chemical reactions , molecular diffusion in rock matrix).

CONCEPTS

Geometrical framework and parameters
Three-dimensional box divided into:
-Hydraulic conductor domains. 2-D features (location, extent, orientation).
-Hydraulic rock mass domains. 3-D features (location of boundaries).

Material properties
Kinematic porosity , (n_e).
Dispersivity (α_L,α_T).
Molecular diffusion coefficient.
Retardation coefficients.

Spatial assignment method

Kinematic:	Deterministic assignment within a domain, - constant
Dispersivity:	Deterministic assignment within a domain, or by a probable density function for particle movement (pdf(p)).
Molecular diffusion coeff.:	Deterministic assignment within a domain
Retardation coeff.:	Deterministic assignment within a domain or by pdf(p)

Boundary conditions

Flow field:	See concepts for groundwater flow.
Mass or concentration:	Mass flux or prescribed concentration of the solute.

Numerical tools
PHOENICS finite-volume code.

Output parameters
Salinity distribution
Flow paths

Scope of work related to the transport of solutes

The tests aimed at estimating transport properties in the rock mass are briefly described below.

At the Äspö HRL a Long-Term-Pumping test (called LPT2) was performed on the southern part of Äspö in 1990 */Rhén et al 1992/.* During this test tracers were injected into a number of boreholes with the main purpose of testing the connectivity of the conductive system. The dilution in the injection sections was monitored and the arrival of the tracers was monitored in the pumped borehole.

During the construction of the tunnel a simple tracer test was performed in hydraulic conductor NE-1 */Rhén and Stanfors 1993, Stanfors et al 1992/.* The purpose was to obtain some indications of the kinematic porosity for planning the grouting before the tunnel penetrated hydraulic conductor NE-1.

Extensive investigations were performed in a conductive structure intersecting the tunnel at approximately tunnel section 500 m, at about 70 m depth below Hålö */Gustafsson et al, 1994; Banwart et al 1995/.* As a part of these investigations, hydro-tests and a tracer test were performed in the conductive structure.

A project called Tracer Understanding Experiment (TRUE) was started in 1995 and the first tracer test was performed in late 1995 */Winberg (ed), 1996/.* The tests were performed in a rock of fairly low conductivity.

The evaluations of the kinematic porosity and dispersivity in the references mentioned above are based on analytical methods assuming radial or linear flow.

To put the evaluations of the kinematic porosity and dispersivity from Äspö in a general perspective we refer to a compilation from the literature on tracer tests in fractured rocks presented by *Andersson /1995/.* The evaluation methods used for these tracer tests were analytical and/or numerical and the evaluated parameters were given as a single value or range for each parameter.

Methods used

Waterchemical composition and properties for transport of solutes were based on:

- Water sampling in boreholes from surface and tunnel.
- Water sampling of the Baltic water and meteoric water.
- Geophysical logging.
- Tracer tests.

Water samples were the base for the interpretation of the distribution of the salinity and other natural tracers in the rock mass. The logging of the electrical conductivity was initially used to interpret the salinity distribution in the boreholes. Tracer tests were used to test the hydraulic connectivity and to obtain rough estimates of the kinematic porosity. *Figure 7-1* illustrates the pre-investigation methodology.

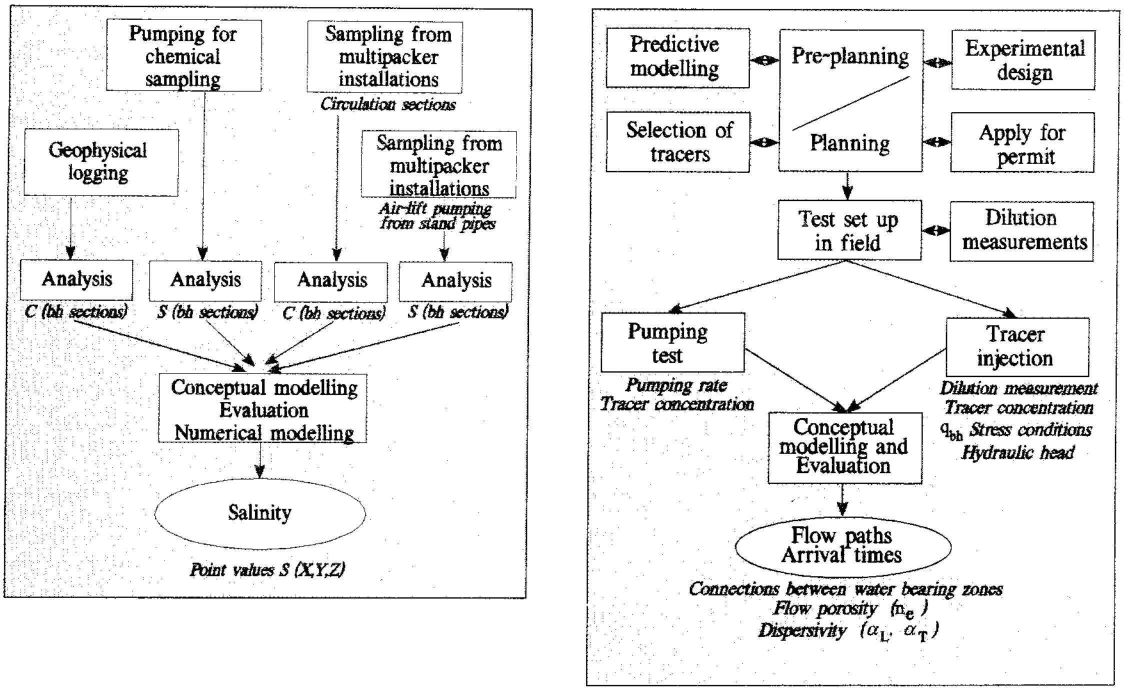

Figure 7-1. Pre-investigation methodology.
Left: Salinity distribution within the rock mass.
Right: Flow paths and arrival times.

7.2 GEOMETRICAL FRAMEWORK

The concepts, used of the geometrical framework are the same as for the groundwater flow shown in *Chapter 5*:

- Hydraulic conductor domains,
- Hydraulic rock mass domains.

See *Chapter 5* for more details concerning the domains. The numerical groundwater flow modelling with PHOENICS code described below is based on the models mentioned in *Chapter 5*.

Hydraulic conductor domains

The LPT2 test confirmed the hydraulic conductor domain NNW-2 */Rhén et al 1992/*. It was shown that there was good connectivity between the injection point and the pumped borehole, both boreholes were assumed to intersect NNW-2. The injected tracer that was intended to show the connectivity within hydraulic conductor domain EW-5 never showed up. It was interpreted that EW-5 was possibly highly fractured and that the test duration was not long enough to show the break-through.

NNW-2 was confirmed by hydraulic tests in the tunnel. EW-5 could not be confirmed in the tunnel, only subhorizontal fracture sets and a few minor subhorizontal fracture zones were found. The present model does not include any hydraulic conductor domain corresponding to EW-5.

The tests in the hydraulic conductor domains NE-1 */Rhén and Stanfors 1993, Stanfors et al 1992/* and the Redox zone */Gustafsson et al, 1994; Banwart et al 1995/* also confirmed connectivity between the points in the interpreted domains.

7.3 MATERIAL PROPERTIES

The material properties for the domains are:

• Advection	• Kinematic porosity (n_e)
• Mechanical dispersion	• dispersivity (α).
• Molecular diffusion	• effective diffusion coefficient (D^*).

(Retardation parameters are not described here as solely generic modelling was done of techniques of how to incorporate retardation in the model. References are shown in *Rhén et al /1997b/*).

The kinematic porosities for some of the hydraulic conductor domains were calculated to 0.002-0.007, assuming radial flow for the evaluation. The dispersivities were estimated to 7-20. The distances between injection points and sampling points in these tests were in the range of 40-200 m. For more details see *Rhén et al /1997b/, Rhén et al /1992/, Rhén and Stanfors /1993/, Stanfors et al /1992/, Gustafsson et al /1994/* and *Banwart et al /1995/. Winberg (ed) /1996/* reports lower values for the dispersivity and kinematic porosity but the rock was also fairly low-conductive.

In some of the numerical groundwater flow simulations performed up to 1995 a kinematic porosity of 0.001 was used for scoping calculations of the mean travel time for particles released in the model.

In the numerical modelling using the PHOENICS code at the Äspö HRL up to 1995 the hydrodynamic dispersion was assumed to be constant or dependent of the Darcy velocity within the model. The hydrodynamic dispersion has so far, using the PHOENICS code, been modelled as $\alpha \bullet L \bullet q$ where α is a dispersivity coefficient, L is the coefficient that can be associated with the cell size in the numerical model and q is the Darcy velocity. Molecular diffusion has been neglected. When the salinity distribution within the model was calculated the dispersivity was assumed to be a constant within the model and not dependent on the direction of flow. The dispersivity within a cell in the numerical model was set at $\alpha \bullet L = 2$. The cells size were 20 m cubes below Äspö. However, a technique was also tried with probability density function controlling the particle movements (pdf(p)) in each cell in the model in order to simulate the effect of the heterogenous medium (see *Rhén et al /1997b/* for overviews of modelling performed).

A linear relationship between the salinity and fluid density was used in the numerical modelling and this variable fluid density was included in the pressure term in the equation of motion */Rhén et al, 1997b/.*

7.4 SPATIAL ASSIGNMENT METHODS

In the numerical simulations performed up to 1995 the kinematic porosity and the dispersivity was assumed to have constant values within the modelled volume.

7.5 BOUNDARY CONDITIONS

Water samples were taken for chemical characterization in corehole sections during the pre-investigation phase are the base for assessing the boundary and initial conditions (conditions before excavation).

The following conditions were assumed in the numerical simulations up to 1995:

Upper boundary:
The salinity of the Baltic Sea was assumed to be 0.7%.
The salinity of precipitation was assumed to be 0%.

Side boundaries:
The salinity is 0.7% at sea level and increases linearly to 1.8% at 1300 m below sea level.

Lower boundary:
Zero flux conditions.

7.6 PREDICTION AND OUTCOME

7.6.1 Salinity field

The predicted salinity distribution in space for natural conditions (undisturbed by the tunnel) and for a few tunnel-face positions during construction were presented in *Gustafson et al /1991/* and *Wikberg et al /1991/.* Details of the prediction was presented in *Rhén et al /1991/.* The predicted salinity distributions for natural conditions and for the final tunnel-face position after construction are shown in *Figures 7-2* and *7-4*. The simulations presented in *Svensson /1991/ and Wikberg et al /1991/* were replotted and are therefore not exactly as the figures presented previously. Due to the interpolation of the simulated results, the salinity field has become less irregular in *Figures 7-2* and *7-4* compared to the initial plots. *Figures 7-2* and *7-4* are based on interpolation of the original data from the simulations. Interpolation was made with a program called *Voxel Analyst* and with an interpolation algorithm called the *Metric method*. It uses the powers of the inverse distance as weight. The salinity distributions for natural conditions and for the final tunnel-face position after construction based on measurements was also estimated by interpolation in three dimensions using *Voxel Analyst*. The interpolation algorithm used for the measured data is a distance-based method, called the *Multiquadric method*. The modelled values at the points for the input data exactly match the original input values, except for some minor truncation errors, and the interpolation function also approximately preserves the gradient inherent in the input data.

The data used are measured values from the Baltic Sea, the properties of the meteoric water (on land), samples from the boreholes made during the pre-investigations (29 borehole sections). Samples were also taken from boreholes made during the construction (19 sections in boreholes from the surface and 18 sections in boreholes from the tunnel). The samples representing the tunnel construction are from the end or after the tunnel construction. Most of the observations are above 600 m depth and also focused below Äspö island, central part of the figures. The observation points for the measured values in boreholes are shown in *Figures 6-10* and *6-11*. Due to this the interpolated values should be considered uncertain below 600 m depth and near the vertical boundaries. The assumed boundary conditions for the total salinity of the box for interpolation were:

Land: 0 mg/l

Baltic Sea: 6008 mg/l

Side top corners of the box, z = 0 m: 6008 mg/l

Side bottom corners of the box, z = 850 m: 18870 mg/l (the values in the bottom borehole section in KAS02 (depth 850 m))

The results based on the interpolation are shown in *Figures 7-3* and *7-5* for the same vertical sections as the ones for the prediction in *Figures 7-2* and *7-4*.

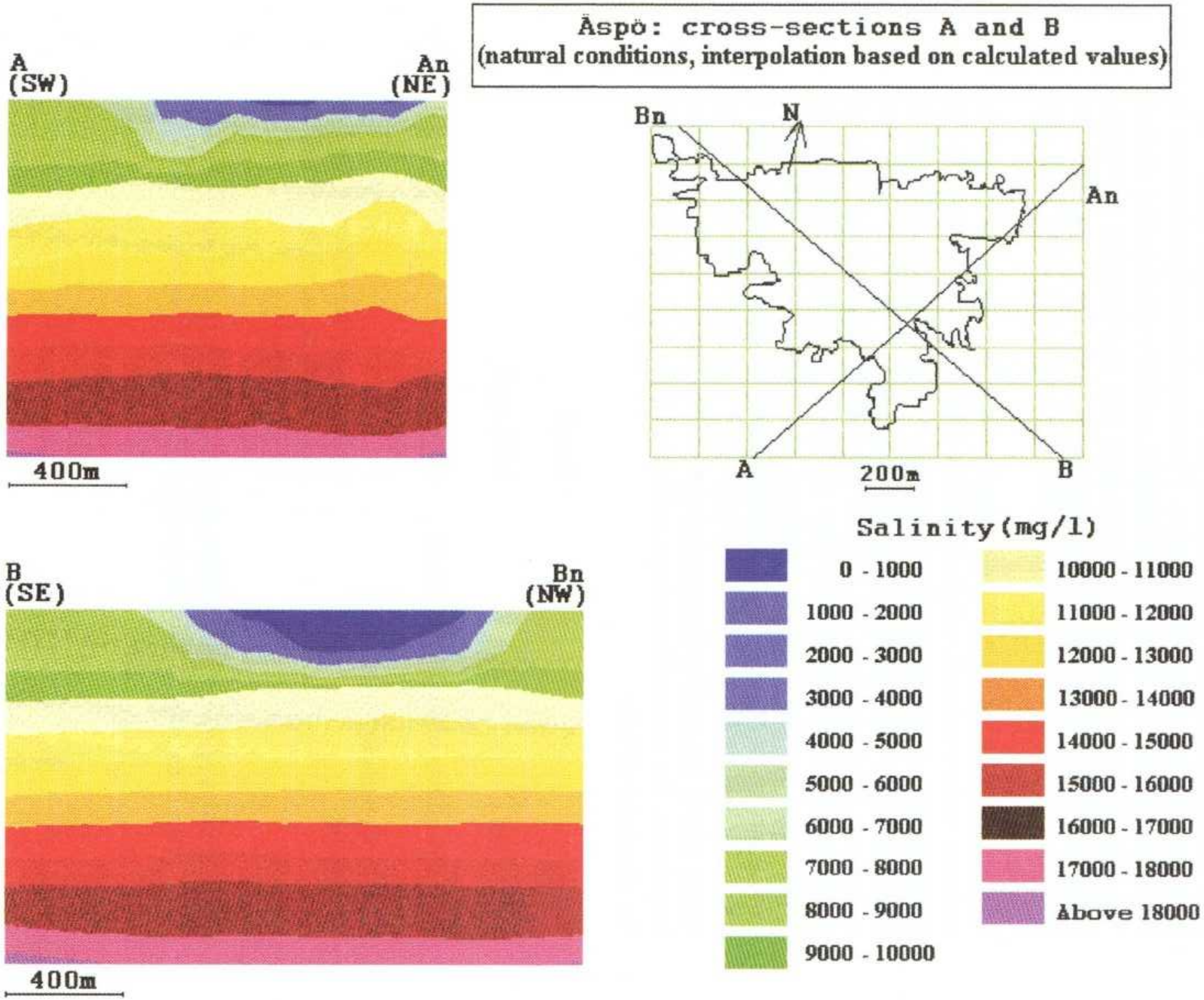

Figure 7-2. *Natural conditions - Numerical groundwater flow simulations. The salinity distribution is shown for two vertical sections, section A (above) and B (below). Salinity is given in mg/l. The maximum depth of the vertical sections is 1250 m, which correspond to the bottom in the numerical model. (Simulations presented in Svensson, /1991a/ and Wikberg et al, /1991/ have been replotted and are therefore not exactly as the figures presented in these reports).*

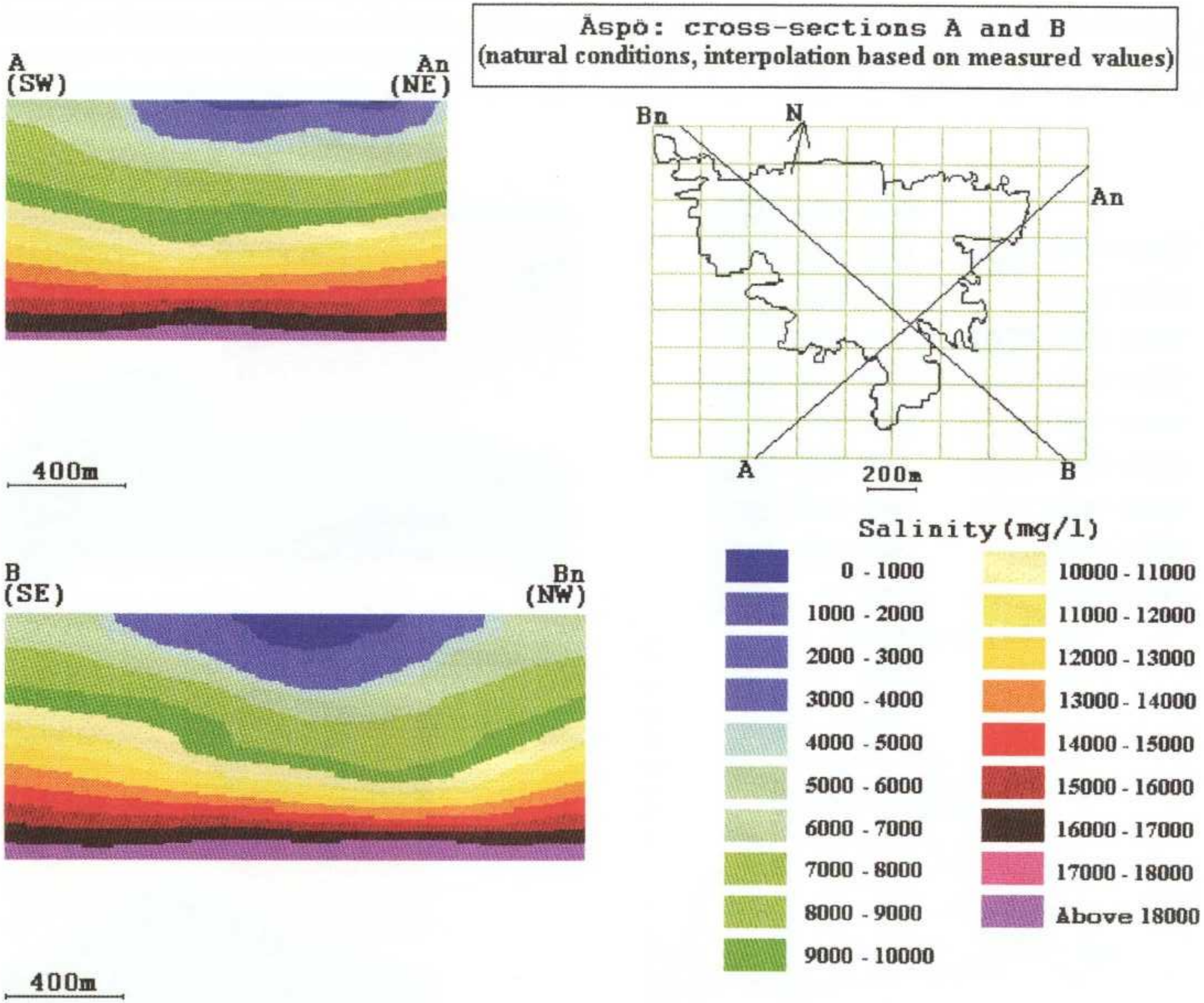

Figure 7-3. *Natural conditions - Interpolation based on the measured values. The observation points for the measured values in boreholes are shown in Figures 6-10* and *6-11. The salinity distribution is shown for two vertical sections, section A and B (below). Salinity is given in mg/l. The maximum depth of the vertical sections is 850 m, which corresponds to the deepest measurement point.*

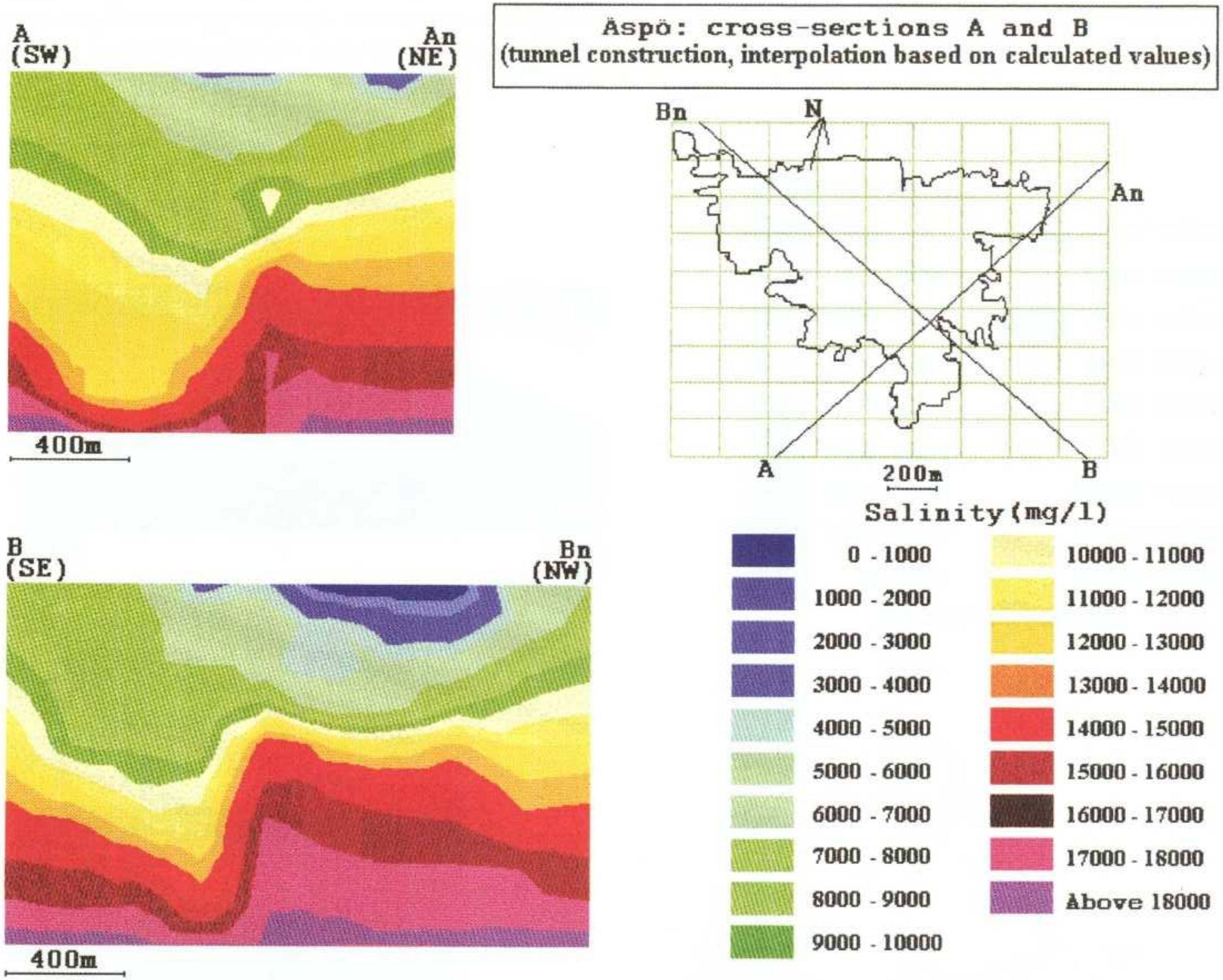

Figure 7-4. *The final tunnel-face position after construction - Numerical groundwater flow simulations. The salinity distribution is shown for two vertical sections, section A (above) and B (below). Salinity is given in mg/l. The maximum depth of the vertical sections is 1250 m, which correspond to the bottom in the numerical model. (Simulations presented in Svensson, /1991a/ and Wikberg et al, /1991/ have been replotted and are therefore not exactly as the figures presented in these reports).*

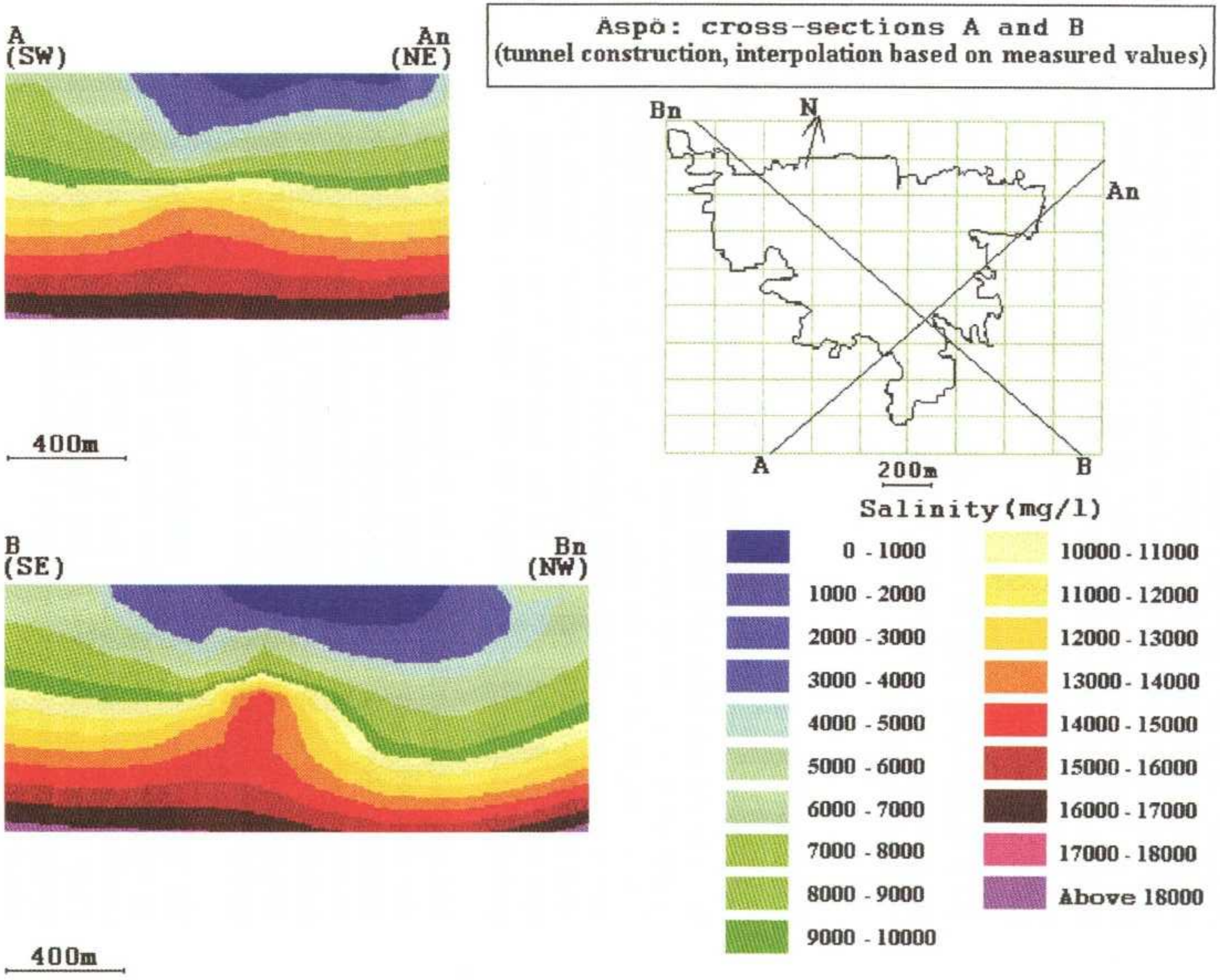

Figure 7-5. *The final tunnel-face position after construction - Interpolation based on the measured values. The observation points for the measured values in boreholes are shown in Figures 6-10* and *6-11. The salinity distribution is shown for two vertical sections, section A and B (below). Salinity is given in mg/l. The maximum depth of the vertical sections is 850 m, which corresponds to the deepest measurement point.*

Changes in salinities were modelled based on the pre-construction *Model 90* and assessing the impact of excavation response on the flow field. Under undisturbed conditions the maximum depth of the fresh water bubble was predicted to be some 200 m *(Figure 7-2)* and the measurements indicate a maximum depth of about 250 m *(Figure 7-3)*. Observations in boreholes from the surface show that water with a salinity of 17000 mg/l under undisturbed, natural, conditions was found at a depth of about 700-800 m. Salinity of 8000-10000 mg/l under undisturbed, natural, conditions was found at a depth of 400-500 m. After excavation of the tunnel, water in boreholes drilled from the tunnel at a depth of about 360 m showed a salinity of about 17000 mg/l. Minor changes in the salinity were observed in boreholes at some distance from the tunnel.

The predictions made using the numerical model also indicated an 'up-coning' of saline water (see *Figure 7-4*). The numerical model, *Model 90*, was a stationary simulation.

Conclusions

Generally, the salinity of the water flowing into tunnel sections and in the boreholes did not change very much during the construction of the tunnel. The salinity of the water flowing into the tunnel changed more than that of the water to boreholes drilled from the surface. In some boreholes along the tunnel the salinity increased considerably compared with the values measured at about the same level before construction in boreholes from the surface. This was also in line with the predictions based on the numerical model. Measured and predicted values indicate up-coning of the saline water in the same range.

Although the predicted flow rates for the tunnel spiral were about twice the measured ones, the predicted salinity distribution was about the same as the measured! However, the predicted drawdown was in the same range as that measured (see *Rhén et al /1997a/*), and the drawdown seems to control the distribution of the salinity. The salinity distribution is more dependent on the pressure field than on the hydraulic conductivity field and is thus easier to predict than, for example, the water flux in the rock.

The *Model 90* was a stationary simulation but due to the different stages of prevailing hydrological conditions since the last glaciation the boundary conditions are changing and may play a role for the present situation at Äspö. There remains uncertainties of how the shore displacement, and also the development of the Baltic sea since the last glaciation, influence the distribution of salinity at present.

7.6.2 Natural tracers

Predictions 1990

In the model presented before tunnel construction was started all hydrochemical information was presented as concentrations of the most important ions and isotopes. Some of them are considered to be non-reactive and thus capable of being used as groundwater tracers. Some manual calculations were done to predict the concentrations of these natural tracers at selected time steps during construction. As a basis for the calculations three different water types were selected, Baltic Sea water, meteoric freshwater and deep saline water.

Scoping calculations with Model 90

With *Model 90* scoping calculations of the flow paths from some of the borehole sections to the tunnel were made. Calculations were performed as stationary simulations with the tunnel face at four positions (about 1450 m, 2500 m, 3100 m and tunnel after construction). Calculations showed that the travel times from several borehole sections on southern Äspö to the tunnel were just a few days assuming a kinematic porosity of 0.001 */Rhén et al, 1991/.*

Evaluation of predictions

During construction the natural tracers were monitored in selected borehole sections at Äspö. At the same time the dilution rate was measured in the same borehole sections. In most cases there were large differences in the flow rates compared with the predictions. The observed rates were generally one to two orders of magnitude lower than the predicted.

Because of the difference in the dilution rates mentioned above, a systematic scrutiny of the separate measurement points was judged not to be meaningful. However, a more important question now is how the enhanced knowledge of groundwater evolution would have changed the way the predictions were made. The present hydrochemistry model includes the definition of five water types ('reference waters') which in varying proportions describe all observations. If this model had been available when the predictions were made, the predicted item would have been the mixing proportions of the reference waters. The observations to be compared with the predictions are:

NE-4 is dominated by sea water, which increased from 44 to 69 per cent during construction while shallow water decreased from 29 to 23 per cent. (Depth below sea level at the tunnel intersection: ~ 110 m.)

NE-3 is dominated by seawater, which decreased from 76 to 69 per cent during tunnel construction. (Depth below sea level at tunnel intersection: ~ 140 m.)

NE-1 is dominated by seawater, which increased from 44 to 76 per cent while the shallow water decreased from 30 to 16 per cent. (Depth below sea level at tunnel intersection: ~ 180 m.)

EW-3 is dominated by seawater, which changed from an initial 43 to a stable 65 per cent with a decrease of shallow and glacial water. (Depth below sea level at tunnel intersection: ~ 200 m.)

NE-2 is dominated by glacial water at all three intersections with the tunnel. The proportion of glacial water decreased from 65 to 30 per cent, 45 to 19 per cent and 47 to 45 per cent respectively during construction of the tunnel. (Depth below sea level at tunnel intersections: ~ 220-350 m.)

NNW-4 is dominated by shallow water in the proportion of some 30 per cent (Depth below sea level at tunnel intersections: ~ 250-400 m.)

With an updated model for the hydraulic conductor domains (*Model 95*) scoping calculations of the flow paths were made. In this case back-tracking of the particles from the tunnel was used in order to trace the origin of the water flowing into the tunnel. The calculations were stationary simulations with no tunnel present (undisturbed conditions) and with the tunnel face at 1475, 2265 and 2874 m. */Ittner and Gustafsson, 1995/.*

The flow paths considered to be of most interest were the ones identified from the LPT-2 tracer test. Data on flow porosity was obtained from the same tracer test.

The general picture of the proportion and the distribution of the 'reference waters' along the tunnel show that there is a general agreement between the observations and predictions.

7.7 EVALUATION NUMERICAL, MATHEMATICAL TOOLS

One purpose of including the transport of solutes in the numerical modelling was to estimate the salinity distribution within the modelled volume, which affects the fluid density and then also the fluid flow (see *Chapter 5*). Salinity was also used as a tracer to study the salinity within the flow field under natural (undisturbed) conditions and during construction of the Äspö HRL.

Another important use of the numerical model was to study flow paths under natural (undisturbed) conditions and during construction of the Äspö HRL in order to trace the origin of sampled groundwater.

Up to 1995 only a few tests had been performed with sorption/desorption of particles on their flow path using the PHOENICS code (see references in *Rhén et al /1997b/*).

A method for calculating the proportions of different water types using the numerical groundwater flow model was tried. The calculated flow field is used for back-tracking marked fluid elements, released around the tunnel or near a borehole section. Back-tracking means that all flow vector components are used with reversed signs. If it is assumed that stationary conditions prevail it is possible to calculate the paths for the water passing the borehole section or entering the tunnel. It is then also assumed that no chemical reactions will take place along the flow path.

It is also possible to visualize the region in the rock mass where most of the particles are at a certain time before entering the tunnel or passing a borehole section. The particle distribution can be shown by an iso-surface for the particle concentration.

It can of course be argued that the flow conditions are transient and will affect the composition with time as water flows into the tunnel. However, it seems to be a simple and fast method (as it is a stationary flow field) to get some idea of the flow paths and the possible origin of the water. As a next step it would naturally be desirable to do transient simulations and release particles at relevant points, or evenly distributed throughout the rock mass. However, it is important to release a very large number of particles in order to calculate the proportions in relation to time. The computer simulations may thus become time consuming.

7.8 EVALUATION OF SITE INVESTIGATION METHODS

Hydraulic connectivity

The tracer tests were useful for testing the hydraulic connectivity between borehole sections assumed to be in a hydraulic conductor domain. Hydraulic interference tests give rather good opportunities to indicate hydraulic communication within a defined hydraulic conductor domain, if the transmissivity is high compared with the transmissivities of the possible hydraulic conductor domains intersecting the tested domain fairly close to the pumped borehole. However, it is pressure responses that are measured at observation points in an interference test and not flow rates. It is possible that a packed off borehole section intersects close to a boundary of a very transmissive fracture. In such a case the interference test indicates good hydraulic communication with the pumped borehole but still the water in the fracture may be more or less stagnant. Thus, in some cases there may be problems when performing a tracer test, but if the rock is highly fractured in the borehole section where tracer is to be injected the risk of problems is probably minimal. Dilution test is a useful method for finding out if a borehole section is in good contact in terms of groundwater flow.

Transport parameters

Site-scale tracer tests can be useful for confirming the connectivity within hydraulic conductor domains. Evaluation of reliable estimates of the transport properties from these large-scale tests seems to be difficult so far.

The tracer tests in NE-1 and the redox zone were rather successful for defining hydraulic connectivity but also for approximately estimating the kinematic porosity. For these cases the test scale (distance between injection sections in boreholes and inflow to boreholes or tunnel) was up to about 100 m and the hydraulic conductor domains were fairly well defined geologically.

The usefulness of some pre-investigation methods is summarized in Table 7-2.

Table 7-2. Presentation of usefulness of different investigation methods. ***/Almén et al, 1994/.***

Subject	**Methods**	**Usefulness**
		Regional, Site scale
Flow path and arrival time	Tracer test	3
Natural tracers	Sampling in percussion boreholes	-
	Sampling during drilling	1
	Sampling during interference tests	3
	Complete chemical characterization	1
	Monitoring of chemistry and the natural groundwater flow in permanently packed-off borehole sections	3
Saline interface	Geophysical logging	1
	Pumping for chemical sampling	3
	Air-lift pumping of packed off sections	2
	Chemical sampling in water circulation sections	3
	Electrical conductivity measurements in borehole sections	1

Very useful = 3 Useful = 2 Less useful = 1 Not applicable = -

7.9 OVERALL EVALUATION CONCERNING THE TRANSPORT-OF-SOLUTES CONCEPTS

7.9.1 Models

Salinity

It was possible to reproduce approximately the salinity field by numerical simulations with the groundwater flow model and the material properties assumed for the transport of solutes. As regards the transport of salt the simple approach used seems to work satisfactorily. However, more realistic descriptions of material properties and boundary conditions should be tested in the future.

Transport parameters and hydraulic connectivity

The LPT2 test was performed on a large test scale, several 100 m, and several hydraulic conductor domains were tested. As a connectivity test it was useful but the evaluation of the transport properties was more difficult. A number of modelling groups used the data from the LPT2 test and tried to simulate the transport, but found it difficult to find a 'unique' solution concerning the transport parameters. The modelling work is summarized in *Gustafson and Ström /1995/* and reported in detail in *Rhén et al /1992/, Hautojärvi /1994/, Taivassalo et al /1994/, Billaux et al/ 1994/, Noyer and Fillion /1994/, Barthelemy et al /1994/, Holton and Milický /1996/, Gylling et al /1994/, Kobayashiet al /1994/, Igarashiet al /1994/ and Uchida et al /1994/.*

Flow paths and arrival times

Flow paths and arrival times were not specifically assessed, mainly because these subjects were not particularly important at this stage. However, it may be concluded that the models for calculation of flow paths and arrival times must be further developed.

7.9.2 Scoping calculations

A summarized evaluation, based on data from comparisons between calculations and outcomes */Rhén et al, 1997a/* is presented in *Table 7-2*. The '+' sign represent the most common parameter result. The results are discussed briefly below.

Groundwater chemical composition and transport of solutes

The combined effect of sparsely made predictions (with only a few points in tunnel and surface boreholes with complete time series of chemical, head and flow data) together with changed tunnel lay-out, revised fracture zones and changed chemical end-members, makes evaluation of prediction reliability cumbersome. However, the overall conclusion is that the predictions made during the pre-investigation as a whole are in accordance with the outcome, although the tunnel breach of zone NE-1 changed the transport of solutes and chemical composition in zones NE-2 and NNW-4 to a larger extent than was predicted. The surface type of waters also penetrated the fracture zones to a lesser extent than expected from the predictions.

Table 7-2. Comparisons between predictions and outcomes ***/Rhén et al, 1997a/.*** **The '+' sign represent the most common parameter result. (+): Results only based on scoping calculations.**

Subject	**Site scale** **Within range**	 **Outside range**	**Comments**
Salinity			
In boreholes	+**		
Saline interface	+**		
Flow paths	(+)		The flow paths in the groundwater flow model do not contradict the groundwater chemical measurements in the tunnel boreholes, surface boreholes or Baltic Sea.
Arrival time	(+)		A few results based on the groundwater chemical measurements in the tunnel boreholes indicate transport times in the same range as estimated using the groundwater flow model.
Natural tracers	-	-	A systematic scrutiny of the separate measurement points could not be made (see text).

** No strict ranges were given in the calculations. However, the results from simulations with two different tunnel skins are here used as prediction ranges and a judgement is made as to whether the results are relatively close to the predicted range (=within predicted range) or not (outside range).

7.9.3 Conclusions

- The multivariate groundwater mixing and mass balance modelling concept M3 seems to be one of the tools that can be useful for the interpretation of the flow paths and transport times. Another tool is of course a groundwater flow model for calculations of flow paths in the rock mass that can be compared to the multivariate groundwater mixing and mass balance modelling. However, there is still much work to be done to improve the integration between the groundwater flow, groundwater chemistry and transport of solutes models. Work is on-going.

- Tracer tests are useful for checking the connectivity within and between hydraulic conductor domains. At a relatively small scale, about 50-100 m, it seems possible to get rough estimates of the flow porosity and dispersivity within a hydraulic conductor domain. At larger scales it is difficult to evaluate the transport properties but the tests can be useful for defining hydraulic connectivity.

- The tests on larger scales may also demand a fairly long test time, involve a large number of observation points for pressure and points for tracer injection. Because of this the large-scale tests also become quite expensive to perform.

- It should be pointed out that few attempts have been made to estimate the transport properties of the rock mass at Äspö HRL sofar. In the next phase of the Äspö HRL a much greater effort will be made on finding useful concepts and parameters for calculations of transport of solutes.

8 EVALUATION OF THE SITE CHARACTERIZATION METHODOLOGY APPLIED AT ÄSPÖ

8.1 INTRODUCTION

The aim of *Chapter 8* is to highlight some topics in the methodology used on the Äspö HRL Project. It includes evaluation of the:

- iterative approach to site characterization.
- multi-disciplinary approach to data collection and interpretation.
- modelling in different scales.

The next section is devoted to important new findings in connection with characterization in conjunction with construction and the following section summarizes the evaluation of subjects of importance for each key issue defined. In the last section our findings at Äspö are summarized and evaluated in the light of the siting factors that SKB applies to the siting of the deep repository for spent fuel */SKB, 1994/.* During the course of this work, a great deal of general experience was gained and reported in *Bäckblom et al, /1997/* and the reader is referred to this report for details.

8.2 EVALUATION OF THE ITERATIVE APPROACH

It is quite obvious that an iterative approach to site investigation is preferred. The iteration should encompass all the activities, not only the data collection (see *Figure 2-4).* Iteration should continue up to a point when there is enough confidence that the known uncertainties are acceptable for the respective steps of design, construction and licensing of the repository. Using the iterative approach, results should become more certain, with time (see *Figure 8-1).* Three important stages in the iterations can easily be defined for the level of understanding and knowledge; 1: at the start of site investigation, 2: at the start of construction and 3: after construction.

The following sections describe some general experience and evaluations, structured as shown in *Figure 2-4.*

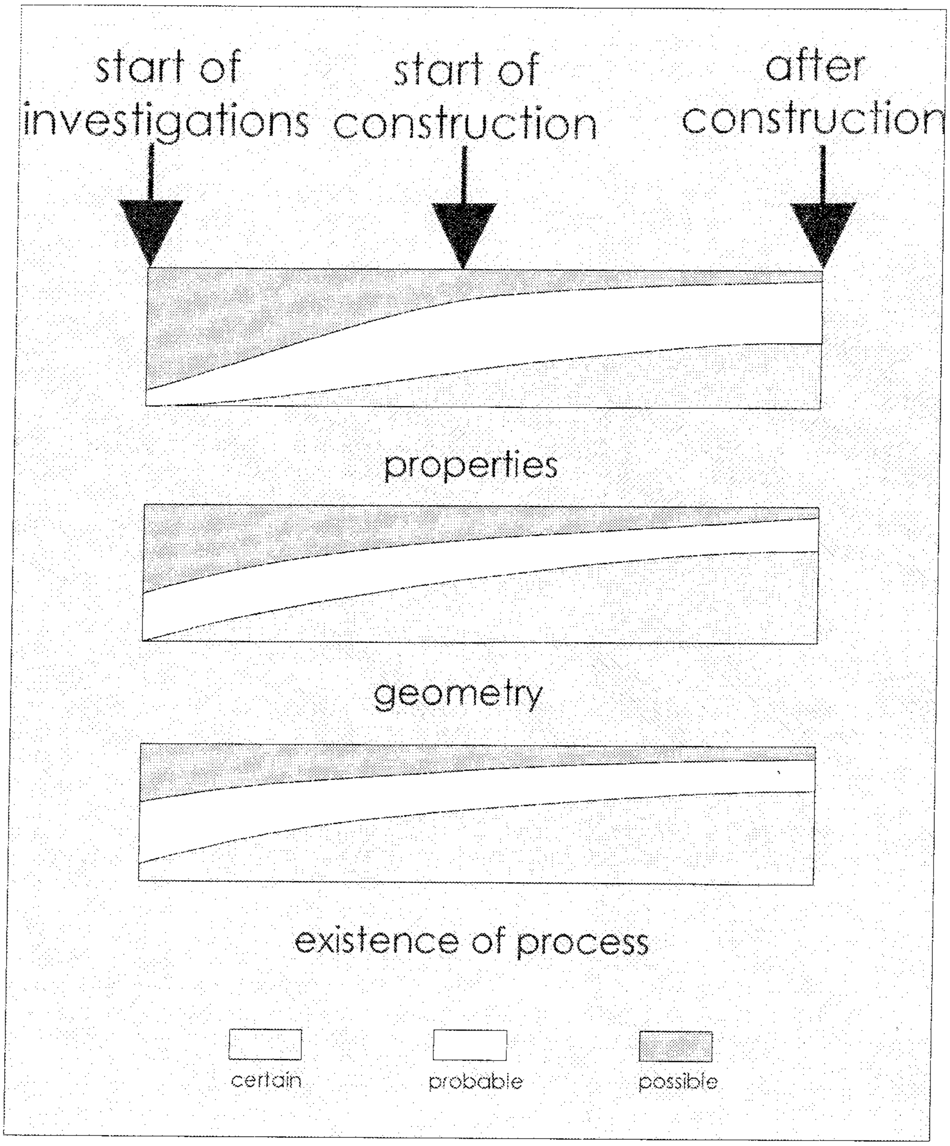

Figure 8-1. The horizontal axis shows how understanding and knowledge is increased with further site investigations. First the existence of processes are found out, then the geometry (e.g. domains of existence, spatial assignment) and finally the properties for the domain are derived. In spite of detailed investigations uncertainties will always exist and these must be taken into account in the design and the performance and safety assessment.

Goals

Time and greater understanding has led to a successive development of the objectives of the Äspö HRL Project */SKB, 1986, SKB, 1989, SKB 1992/.*

The Äspö HRL was launched with a general thought that a laboratory is an important tool in driving the overall programme forward. The laboratory can be used to test and develop methods and technology before being applied to a real site. This includes site characterization technology, construction and handling methods, and long-term pilot tests of parts of a repository.

The driving force for defining the site investigations were the data need for safety analysis and for design and construction of the laboratory. The set of data needed has however successively developed. A common basis for the Äspö programme has been *that the site investigations shall provide a good understanding of the site and a sufficiently comprehensive data set to be able to handle various issues during construction.* Within the project a detailed list of subjects for the site investigations were developed. Based on the experience from Äspö a general site characterization programme is being developed by SKB. This programme will address (in as great detail as is reasonable in advance with no or limited knowledge of the specific site) those measurable parameters that are relevant to safety as well as to design and construction. The parameters chosen by the Äspö project are mainly a part of those defined in the site characterization program under development.

Data collection

A multi-disciplinary approach was used in the data collection. Several improvements in methods have been achieved during the pre-investigation and construction phases. Examples of significant technology developments during the Äspö project for data collection are the telescope shaped borehole design, technology for dilution measurements to measure groundwater flow, the flow-meter tool for identifying water conductors, and the on-line monitoring network of boreholes. However, there is still a need for further improvement */Bäckblom et al, 1997/,* and such developments are in progress. Examples are a positioning system for measurements in boreholes, reversed flushing during drilling to minimize groundwater contamination and methods to simplify orientation of fractures in boreholes by digital down-the-hole TV. Further developments are for example a need for improved groundwater sampling technique and flow meter logging in the upper part of the telescope shaped boreholes.

The independent review of the data from the pre-investigation data in the SKI Site 94 Project */Geier et al, 1996/*, confirms many of our own conclusions, especially with respect to the usefulness of the previous data base management system. As a result of the Äspö findings a new data base system - SICADA - has been developed. Large amounts of data are collected and it is important to have a good data base structure including some references to more details about the data, for example descriptions of measurement techniques.

Data collection (with exception of reflection seismics) was adequate to make conclusive statements of importance for engineering purposes. Data have been enough in quantity and of good enough quality to show the existence of several important processes in the rock. The geological models and geometrical framework were in general reliable. But the amount of data was not, as expected, adequate for deterministic descriptions of minor discontinuities in the rock. Nor has the data quality been adequate for precise determination of the primary stresses. For many parameters the natural variability makes it only feasible to derive a stochastic distribution of the parameter in question.

In general, parameter values can be derived with reasonable effort. However, it can be very time consuming to show the non-existence of processes or features like fracture zones, especially when only one method provides an indication that the process/feature exists. A practical example is where analyses of reflection seismics indicated subhorizontal fracture zones at Äspö, which conformed to the general understanding of the geological setting of the region where such subhorizontal zones exist. A great deal of effort was needed to resolve the relevance of these seismic indications. It was found that the seismic results did not correspond to any subhorizontal zones of importance down to about 500 m depth. The two gently dipping fracture zones (less than 1 m wide) mapped in the tunnel are probably too narrow to be indicated by the seismic reflection used at Äspö but today the reflection seismics technique has developed and probably give better possibilities to detect subhorizontal fracture zones compared to a few years ago.

Analyses

The analysis part of the site investigations is at present the most complex one. Based on previous experience and data collected at the site one or several conceptual models should be chosen to describe a process. Each conceptual model presents its own needs for data and interpretation of data. However, when a conceptual model has been selected, the data need and interpretation of data become more straightforward. The data collected should also allow alternative interpretations based on different conceptual models. It should also be pointed out that inter-disciplinary interpretation is vital as supporting evidence for certain models.

There are sometimes conceptual uncertainties of a general nature that are complicated to analyse, like the scale-dependency of parameters. Our approach to scale-dependency of the permeability of the rock mass was to perform tests on several measurement scales. Further, several conceptual alternatives are likely to be viable for models of hydraulic conductivity, retardation, etc. There is a need for a dedicated effort to consistently present results with error bounds representing both measuring accuracy, parameter variability and conceptual uncertainty.

Our approach to dealing with the geometrical complexity of the rock was to distinguish between deterministically assigned geometry and properties and stochastically assigned geometry and properties. This separation has been of value to treat the complexity of the rock *(Figure 8-2)*. There will always be a choice to be made as to what should be described deterministically and what should be described stochastically. This decision is dependent on the purpose, scale, availability of data, etc.

In-depth analyses of the results can be hampered by the allocation of insufficient time. Thus, it is imperative that the time targets of the overall site investigation permit careful analyses and co-interpretation. There is a need for in-depth analyses not only to describe how things are, but also *how things cannot be* as well. However, there is a general advantage using the iterative updating approach to analyses and modelling, i.e. starting with the simplest possible model and making it more sophisticated if necessary. Thus, unresolved questions can be taken care of in the next iteration.

Simple rules used for the data collection and subsequent analyses were dogmas like 'Do not collect data at a greater rate than we can document and evaluate', 'Data will only be collected if there is a client/customer who will bear responsibility for evaluating it'. These simple rules should be remembered during site characterization.

It is also a great advantage if there is an interactive 3-D CAD system available for interpreting results, integrated modelling, visualization and transformation of relevant geometrical information into numerical groundwater flow models, for example.

Models

For Äspö the intended use of modelling was to develop predictive models to forecast conditions to be measured during construction of the Äspö facility. To obtain a simple overview of models (concepts, data) a model format was developed */Olsson et al, 1994, Chapter 2/* using principles which are employed in this report. *(Chapter 3-7).*

Inter-disciplinary modelling work should be performed continuously throughout the characterization work to ensure that models are consistent. Investigations are made in steps and after each step integrated geological, hydrogeological and hydrochemical models are established. These integrated models should be the base for planning further investigations. It is also essential that enough time be reserved for analysis of collected data and updating of the models between each step. It is also of major importance at an early stage in the investigations to select an appropriate, consistent nomenclature for descriptions of, for example, fracture zones, lithology and groundwater chemistry.

Predictions

The model (of a process) consists of the model elements; *geometrical framework*, material properties, *spatial assignment* and *boundary conditions*, see *Table 2-1*. Now for a real case, *data,* will be needed for the four elements of the model. If necessary a *numerical* or *mathematical tool* that handles the processes and features should be chosen as a prediction tool. And, finally, there is a need to select *output parameters* that satisfy the *purpose* of the model. It is ideally the output of the model that should be predicted. This implies that the predicted output also can be measured in a useful and feasible manner. If this ideal situation can not be arrived at, the alternative is to estimate the parameters for each model element, for example the material properties.

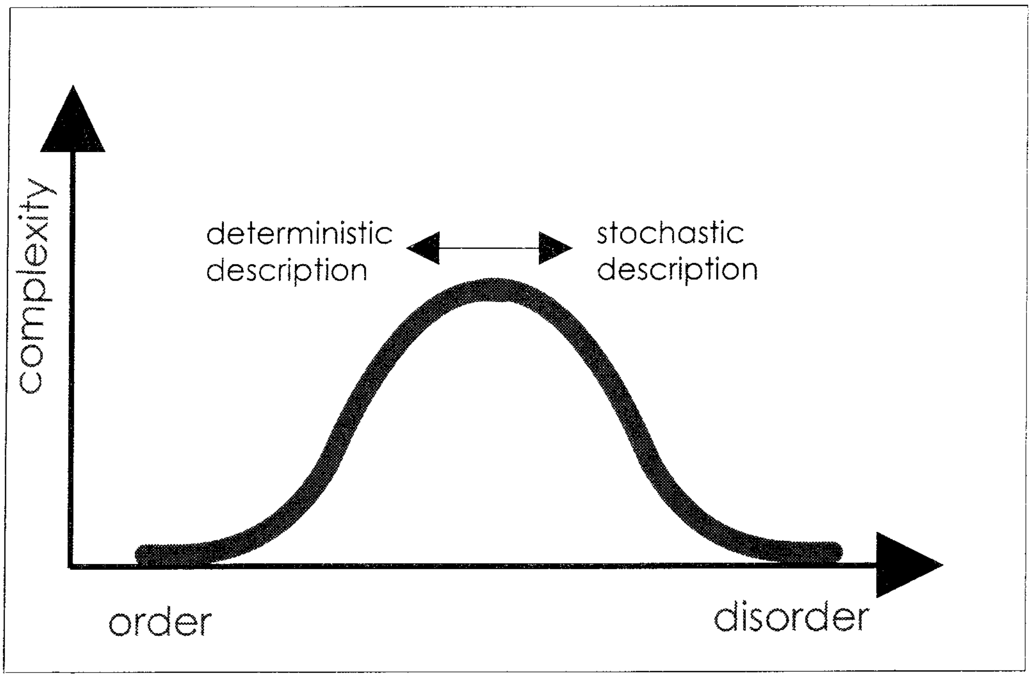

Figure 8-2. Complexity exists between order and disorder. In general it is easier to analyse and describe a completely ordered or completely disordered system. Complete geometric disorder (chaos) is a random system requiring few parameters for description. The completely ordered system is also easy to describe with few parameters. At Äspö certain subjects are described using a deterministic approach; other subjects are described using a stochastic approach, first using non-correlated data. Application of spatial correlation of the stochastic data makes models more complex. The study of complexity is itself a general scientific discipline and the reader is referred to /Nørretranders, 1994/ for a popular presentation.

The groundwater flow models can be tested with data from large scale interference tests and drawdown by the facility constructed. However, with groundwater flow models, for example, we calculate the flow distribution, which can not readily be measured in the case of a large volume. Therefore sub-sets of the model, as the geometrical framework, material properties, etc. are tested using the prediction-outcome approach in order to obtain confidence for the model.

Different approaches have been taken for the predictive work. For parameters where many samples will be collected it is possible to calculate an estimate of the mean and variance of a parameter. The mean and variance of a population can be estimated for each investigation stage and while the data sample is getting larger and larger the confidence in the derived statistical distributions is increasing. Where few data will be collected, a lower level of confidence can be used. Some geological predictions were made using a 60% level of confidence. Sometimes expert judgements were made and only possible ranges of parameter values were given. There are also deterministic 'yes-no' predictions to evaluate, like whether a major fracture zone exists or not. For some of these predictions no uncertainty really can be accepted. There should, for example, be no uncertainty regarding reducing conditions in the groundwater at a virgin repository site at repository depth. It will also not be practicable to find a major, water-conducting fracture zone intersecting for example the hoist shaft. In general designers tend to ask for determinism, while safety assessors can meet their needs by stochastic models.

Predictions of lithology, material parameters like hydraulic conductivity, fracture properties and primary stresses are more transparent if there is a clear distinction between measurement accuracy and uncertainty due to natural variability. It is also advisable that a predicted range should be based on the use of different methods for sampling in the different investigation stages. At Äspö hydraulic tests for practical reasons were made with different test-section lengths in the pre-investigations and during the construction. Another example is that rock stresses were determined using different methods in the different phases. Using different methods and different measurement methodology during the pre-investigations and underground investigations causes uncertainties of how to compare the results. This type of uncertainty can of course be limited provided there is a consistency of scales and methods chosen for surface and underground investigations.

The advantage of the systematic use of predictions as a tool to test understanding and knowledge is that it puts clear demands on systematics of the work. The conceptual model(s) must be chosen, data need and means of the updating observations decided. The approach also stresses descriptions of previous results for comparison with the updated results.

The prediction-outcome approach has its advantages, but also some drawbacks. Data collection can be focused too much on finding data in pre-determined spots for which data have been predicted. It is also only possible to focus on the concepts where it is known to be possible to acquire new data iteratively during the construction phase, which can narrow the search for new or alternate concepts.

Evaluation of models

The comparison of predicted parameters with outcome can lead to several explanations and therefore it is also a need to scrutinize the underlying assumptions and processes so that predictions can be defended as being within the range, indicating a reliable model.

The outcome can also be outside the range for several reasons. Wrong conceptualization and also previously unknown (new) processes or features are possible reasons. Previously known processes (features), not taken into account, but which, with hindsight, should have been taken into account in the conceptualization can also be a reason. Misinterpretation of data, incorrect data analyses, insufficient data sample not taking into account natural variability is also plausible. There is of course the difficult aspect of treating the case when predictions are within range, but using a model based on wrong assumptions.

What now is important to bear in mind is that a prediction-outcome approach is only a tool. It is a tool useful for planning, transparency and documentation that simplifies evaluation of model and method usefulness and feasibility. An essential part of the model evaluation is the careful scrutiny of the underlying processes and incorporated assumptions.

Evaluation of methods

Evaluation of methods includes the general investigation approach, the systems for data collection, analyses, calculations, etc. To find out the feasibility of methods, the project has tried to keep a steady pace and thereby eliminating methods and methodology that were impracticable.

A few examples to illustrate that said above: Orientation of cores was not done as much as planned originally due to the low feasibility of the method chosen. Development of digital down-the-hole TV equipment is now a preferred method to obtain a base for fracture orientation. Hydraulic measurements by flow logging (spinner) were introduced due to their usefulness and low cost. Calculations of groundwater flow were performed using a finite volume code (PHOENICS) which at that time was much more versatile than any of the finite element codes.

In the site characterization for a deep repository methods should only be used that have previously been shown to be useful and feasible in practice. At Äspö, however, part of the exercise was to sort out methods that were not useful or not feasible for investigations of rock during pre-construction and detailed characterization in conjunction with construction. If new methods are to be considered in the site investigations for a deep repository, the Äspö facility provides excellent conditions for such tests prior to application at the real site.

It is also important to have a good QA of the methods and that the methods and the measurement accuracy are well documented. Each test should also be well documented in order to facilitate better possibilities to evaluate the raw data in a later stage of the investigations. The QA has improved during the investigations and for example a number of QC documents for several of the investigations have been written. The QA and QC of the data base has also been improved.

8.3 MULTI-DISCIPLINARY APPROACH TO DATA COLLECTION AND INTERPRETATION

Inter-disciplinary work should be performed throughout the investigations to ensure model consistency. To facilitate integration, only four principal investigators, with a broad responsibility, were involved in the science management.

Data collection

Direction, depth, inclination and surface co-ordinates of boreholes were decided in consensus. It was also, more or less taken for granted, that tests for several disciplines should be conducted in all boreholes, to avoid 'the geologist´s hole', 'the chemist´s hole'. The advantage is that several types of observations are collected for the same rock volume, allowing co-interpretation of geology, rock stress, hydrogeology and groundwater chemistry. Borehole design and the test sequence were planned in consensus, maximizing the amount of possible information for each hole. Pumping tests for hydrogeology were planned to allow for sampling of the hydrochemistry as well.

Modelling

In the early phase of the investigations, all data collected were used to support the development of a reliable geological-structural model. The geological, geophysical data were compared with hydraulic responses and the chemistry of the groundwater to decide the discontinuity models. The lithological model was used as a basis for division of hydraulic domains as well. Data for the salinity of groundwater was used to check the groundwater flow model. The model was then used to calculate the flow field to check the groundwater chemistry mixing models. Rock stress measurements are also useful for comparison of the principal direction of the hydraulic conductivity tensor with the rock stress tensor. There is a strong and direct coupling between the geological model and the rock mass classification used to assess excavation stability.

The use of boreholes with common observation locations also simplified co-interpretative work when model updating was done. It is thought that the value of common boreholes overrides the possible disadvantages with inter-disciplinary test deficiencies in the common holes.

8.4 EVALUATION OF MODELLING TO DIFFERENT SCALES

Rationale

One of the early decisions taken by the project was to make models on several scales, */Bäckblom et al, 1991/* (see *Figure 2-1*) as it was thought that models on these different scales would be feasible for the real deep repository. The regional scale >> 1000 m forms a basis for later more detailed investigations. Assessments on a *regional scale* can be used to select possible suitable sites for the repository, to define areas of recharge and discharge and to provide the overall tectonic pattern. The *site scale* models 100 - 1000 m can be used to define major fracture zones and/or major flow paths. These investigations will provide guidance on the depth at which the repository should be placed as well as delineating a potential repository volume. Models on this scale are also used for computing far-field groundwater flux and nuclide transport through the repository and to the biosphere. *Block scale* assessment 10 - 100 m will be used to position deposition tunnels and later to position canisters. The *detailed scale* 1 - 10 m defines the hydrogeological, chemical and mechanical near-field to the canister. By proper positioning of the canisters it will be possible to influence the overall safety of the repository.

Regional scale models

The regional scale model shall provide information useful for selecting potential sites for the repository. It shall also provide enough data for setting up groundwater flow and groundwater chemistry models in a large scale. These models are needed for the general understanding and evaluation of the present and past processes and have to be used to assess the boundary conditions for the site model.

Fairly limited investigations were performed during the pre-investigation phase. Airborne geophysical measurements and lineament interpretation were the base for the regional model. Groundwater sampling, geophysical logging and hydraulic testing in shallow percussion boreholes and a few cored boreholes were used to detail the regional model towards depth. The data was sufficient to select the site for the laboratory but was later found to be insufficient for the understanding and modelling of the regional area with respect to groundwater flow and groundwater chemistry. Supplementary investigations during the construction phase of the laboratory (drilling of one very deep borehole and some ground geophysics investigations traversing a few fracture zones) gave a better insight in processes and properties within the regional model based on the chemical groundwater composition and distribution of hydraulic properties towards depth. However, it is likely that the investigations within a regional area have to be somewhat more extensive than what were made for the Äspö HRL to get a better confidence of the boundary and initial conditions, mainly hydraulic and groundwater chemical but also on the properties of the rock mass in a regional context.

Site scale models

One important issue on the site scale is to find a large enough rock volume to host a repository. The rock at Äspö is more heterogeneous than expected for a deep repository and the number of fracture zones is high. The simple design criterion for the laboratory was to position the spiral so that it was bordered by major fracture zones and not cut by major zones. The investigations at Äspö were adequate in this respect. The investigations at Äspö provide confidence that major fracture zones and their geometries can be known based on pre-construction investigations.

The major fracture zones and their properties were also quite correctly modelled with respect to geological character and hydraulic transmissivity which provides confidence that the pre-construction models also will be useful for performance assessment purposes.

Minor fracture zones and their stochastic behaviour were learnt on the basis of pre-construction investigations and there is confidence that such features will in future site investigations be described in a stochastic sense.

The potential host rock for a deep repository and its groundwater chemistry should also in general be in a reducing state. This was confirmed early in the investigations and further established during investigations in conjunction with construction.

The potential host rock for a deep repository should also in general provide mechanical stability. There is general experience in Sweden that mechanical stability is usually achieved even for very large depths. There is, however, also evidence of local rock burst problems very close to the surface. At Äspö experts judged that some possible rock burst problems would only occur in the greenstones. No indications of rock burst were collected and, thus, the overall expert judgement of mechanical stability at Äspö proved to be correct. However, relevant data to make these judgements are normally scarce and scattered due to large natural variability and model and parameter uncertainty.

Block scale

At Äspö predictions at block scale were basically stochastic for subjects like rock composition, number of rock boundaries, single open fractures, etc. Sampling of data to test these predictions were then conducted in 6 blocks with pre-determined locations along the tunnel. This approach may be questionable as it might have been - due to the natural variability at the site - more reasonable to sample over larger rock volumes to compare sample statistics prior to and after construction. The block scale assessments are of course of relevance for the near-field performance assessment. The findings at Äspö provided statistics of properties on a block scale. However as a 'prediction' exercise the results on a block scale for a pre-determined block in the spiral are typically outside the predicted range, basically due to the lithological inhomogeneity. Thus, for a repository it is of value that the block scale is homogenous to simplify confidence-building for the near-field models. The layout of deposition tunnels should only be preliminary, based on the pre-construction investigations and fixed only after data from the detailed characterization. It is possible that more attention to near-field models in the pre-investigation could have emanated in more precise models. The development of the Baymar approach to describe natural variability */Rosén, Gustafson, 1996/* is a step in the right direction.

Detailed scale

Limited work was conducted to make predictions in four lithologically homogeneous rock blocks situated within volumes used for the block-scale predictions. The observations are considered to be more in line with the predictions compared to the block scale, certainly due to the fact that the predictions were made for the general characteristics of each lithological unit at southern Äspö. The predictions on the 5 m scale were made on generic blocks of each lithological unit, but the block on 50 m scale was defined in space.

8.5 FINDINGS DURING THE DETAILED CHARACTERIZATION IN CONJUNCTION WITH CONSTRUCTION

The **main finding during the detailed characterization is that the pre-construction models are basically confirmed.** The models have of course grown more detailed as the data base was increased.

1. Precise geometrical information on the fracture network and distribution of the lithology has been improved in the near-field to the tunnel *(Chapter 3).*
2. The expanded data set on the stress field has shown that the range of the values of maximum horizontal stresses is larger than previously estimated *(Chapter 4).*
3. There is now greater confidence in the nature, geometry and properties of the water conductors, like major fracture zones, minor fractures zones (fracture swarms) *(Chapter 5).*
4. Data now permits the hydraulic conductivity to be treated as a tensor with anisotropy *(Chapter 5*).
5. The detailed description of the conductive fracture network has been considerably improved *(Chapter 5).*
6. Biological processes have been shown to be important for the control of redox conditions in the rock *(Chapter 6).*

Further, several improvements in underground site characterization have been made and these will be reported in a separate SKB Technical Report (in progress). In this context it can be mentioned that it is expected that the detailed characterization from tunnels in a repository will make the models more detailed but also that the confidence in the models will increase. Some of the results above can serve as examples of expected model developments.

8.6 EVALUATION OF SUBJECTS OF IMPORTANCE

Table 8-1 summarizes findings with respect to the main 'subjects' defined for each of the 'key issues' defined by the Äspö project. It treats the present level of the general scientific understanding, the site-specific knowledge that has been arrived at Äspö and also the usefulness and feasibility of models and methods.

Table 8-1. Summary table outlining subject resolution for pre-investigation methods with respect to scientific understanding, site-specific knowledge at Äspö, usefulness of results and feasibility of methods.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
	Understanding is the 'problem-solving capacity beyond current practice', the ability to grasp abstract concepts, detect and explain unfamiliar errors. If there is a general scientific consensus of the basic principles and approaches the understanding is said to be well established.	Knowledge is 'memorized information', such information that can be readily retrieved from reports, data bases, etc. The degree of knowledge reflects the comprehensiveness and generality of the data base for Äspö. Here the situation prior to construction is considered.	Usefulness, applicability and relevance of models and results to the site investigations for a given purpose (deep repository). The degree of fulfilment of data and analysis requirements.	Ability to collect, analyse and apply data and models in an efficient and timely manner.
GEOLOGY				
Major (subvertically dipping) fracture zones	The mechanisms behind and appearance of major fracture zones are understood.	The knowledge of most of the important major fracture zones in the target area was well established before the excavation of the tunnel started	The positions and character of the major zones are of paramount importance for groundwater flow, transport of solutes and design and construction.	Feasible methods for identifying and characterizing major zones from surface are well established.
Subhorizontal fracture zones	The mechanisms behind and appearance of fracture zones are understood.	The frequency and importance of subhorizontal fracture zones in the Äspö area is low.	If there are subhorizontal zones they may be important for groundwater flow and transport of solutes and design and construction. Relevant for deciding repository depth.	To prove non-existence based on available geophysical methods has shown to be a difficult task.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
Minor fracture zones	Our understanding and the character of minor fracture zones is established.	The orientation and frequency of minor fracture zones are known. The location of specific zones at depth is incompletely known.	The properties of minor zones are important for calculating ambient groundwater flow and nuclide retention. They are also of importance for laying out tunnels at repository depth.	Feasible surface methods to determine property distributions exist.
Small-scale fracturing	The mechanisms of the development of the fracture system in relation to time is known through our knowledge of the geological history of the area. Our knowledge of the geological fragmentation has grown considerably.	The fracture system distributions mapped at the surface have shown to be persistent also at depth. Our knowledge of the geological fragmentation has grown considerably.	Fracture data are important for groundwater flow and nuclide retention and for assessing rock stability.	Fracture mapping methods are well established. Some bias between data collected in boreholes and collected in the tunnel. Need for triple barrel coring to obtain details of fracture zones.
Lithology	The development of the lithology in relation to time is known through our knowledge of the geological history of the area, cf. above.	The occurrence and properties of all major lithological units at Äspö are well known.	Lithology determines to some extent geochemical, hydrogeological and mechanical properties of the rock.	Analysis methods and classification methods are well established.
Lithological distribution	The development of the rock distribution in relation to time is known through our knowledge of the geological history of the area.	The rock distribution at the surface is well known. At depth a probability distribution of rocks can be established. The local variability is uncertain.	The rock distribution determines to some extent the geochemical, hydrogeological and mechanical properties of the rock volume.	Methods for predicting the deterministic spatial distribution of minor rock units in a complex rock mass are not available.

	Scientific understanding	**Site-specific knowledge**	**Usefulness**	**Feasibility**
ROCK STABILITY				
Mechanical properties	The properties of crystalline rocks are generally understood. Understanding of the influence of scale has to be developed.	An adequate knowledge for construction purposes of the properties of Äspö rocks was established. The spatial variability of parameters was under-estimated.	Mechanical properties of rocks are vital for rock-mechanics analyses.	Methods for laboratory characterization of rock type properties are well established. Methods for characterization of mechanical properties of fractures surfaces and fracture zones are not well established. Methods for assessing spatial distribution are not mature.
Rock stress	The regional stress distribution and its reasons are understood. Local variability is less understood.	Adequate knowledge of the direction of the stresses. Maximum horizontal stresses exhibit high variability.	Rocks stresses are vital in analyses of mechanical stability.	Methods for measurement of rock stresses are established, but results indicate needs to further develop the methods. Methods for assessing spatial distribution are not mature.
Rock quality	The rock quality classification system used (RMR) is well established with a comprehensive data-base of case studies.	An adequate classification for construction purposes was established before construction.	Rock classification is of great importance for design and construction planning.	Methods for classifying rock quality are well established. Methods for assessment of spatial distribution are not mature.
Rock burst	The mechanisms behind rock-burst are not well understood.	No rock burst occurred. Slight probability of rock burst was predicted.	Rock burst is of great importance for construction and operation of the repository.	Methods for predicting rock burst are not mature.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
GROUNDWATER FLOW				
Major water-bearing zones	The major water-bearing zones are all related to the major fracture zones. The mechanisms behind these are understood.	The knowledge of all major water-bearing zones in the target area was well established before excavation of the tunnel was started. Knowledge of the variability within zones is incomplete.	The position and character of the major water-bearing zones are of paramount importance for modelling groundwater flow and nuclide retention and for repository layout.	Methods for identifying and characterizing major water-bearing zones from the surface are well established.
Minor water-bearing zones	The minor water-bearing zones are all related to minor fracture zones or single interconnected fractures. The understanding of these is established.	The orientation and frequency of minor water-bearing zones is known. The location, extent and properties of specific zones at depth is incomplete. Knowledge of the variability within zones is incomplete.	The positions and properties of minor zones are important for groundwater flow and nuclide retention and for detailed repository layout.	Surface methods for determining the statistical distributions of frequency, length and transmissivity are available.
Hydraulic conductivity of the rock mass between fracture zones	The basic theory behind the conductive properties of fractured rock is established. Understanding of the influence of test scale, correlation structure and anisotropy is incomplete.	Statistical distributions of the hydraulic conductivity of Äspö were adequately established.	The hydraulic conductivity distribution is important for groundwater flow, nuclide retention and for laying out tunnels and canister positions.	Surface methods for determining the property distribution of hydraulic conductivity exist, but anisotropy make the evaluation of the results more difficult. Methodology defining correlation structures should be improved.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
Boundary conditions	The character and influence of boundary conditions is sufficiently understood.	Our knowledge of the boundary conditions at Äspö is adequate for the purpose of construction-related influence. Knowledge of boundary conditions for regional models and the distant future (> 10 000 years) is incomplete.	The boundary conditions are important for groundwater flow and transport modelling.	Boundary conditions can be assessed by generic data supported by topographical and salinity data. Regional models can be used to define site-scale model boundary conditions.
Groundwater flow models	The scientific basis for groundwater flow models of different approaches is established.	The data base for Äspö is adequate and tested for groundwater flow modelling by different approaches.	The groundwater modelling performed in the Äspö project gave adequate predictions of groundwater pressures and inflow during construction. The inflow is, however, also dependent on the grouting performed.	The assessment of data for the numerical models, and the modelling itself were found to be feasible for a range of different approaches. Assessment of inflow reduction due to grouting was made by expert judgement which may be unsatisfactory.
Pressure around tunnel	The part of the pressure variations around the tunnel caused by variable conductivity are understood. The influence of stress changes, two-phase flow, Excavation Disturbed Zone (EDZ) and grouting remains to be fully explained.	The pressure variation predictions outside the tunnel were within range. The variability of the pressure a few metres from the tunnel walls is large.	Basis for stability and sealing assessment. Parameter of interest when testing the groundwater flow model.	Static pressure distribution can be predicted by numerical modelling with a stochastic continuum or discrete fracture network approach. Calculations are uncertain due to the influence of stress changes, two-phase flow, Excavation Disturbed Zone (EDZ) and grouting. The pressure around the tunnel can be measured, but a large number of measurements are required.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
Flow into the tunnel	Flow into the tunnel related to variable conductivity is understood. The influence of stress changes, two-phase flow, Excavation Disturbed Zone (EDZ) and grouting remains to be fully explained.	The predicted flow into the tunnel was within range. The influence of grouting was estimated by expert judgement.	Flow into a tunnel is a basis for repository design and thus safety during the post-closure period and useful for GW-flow model calibration.	Flow distribution into the tunnel can be predicted by numerical modelling with a stochastic continuum or discrete fracture network (DFN) approach. Calculations are uncertain due to the influence of stress changes, two-phase flow and grouting. Flow into the tunnel can be measured well but dams of good quality are quite expensive and it is difficult to make measurements close to the tunnel face.
Point leakage into the tunnel	The conductive elements of the rock are basically understood. The influence of stress changes, two-phase flow, Excavation Disturbed Zone (EDZ) and grouting remains to be fully explained.	Our knowledge of the actual flow distribution for a range of gradients is small.	The flow distribution in the rock mass is a parameter for calculating nuclide retention.	Measurement of point leakage is feasible only at rock faces, but the flow distribution is biased compared with the flow within the rock.
Flux distribution	Detailed flux distribution within small volumes of the rock is not understood, but large variability is expected.	Attempts to measure local fluxes show orders of magnitude differences from predictions.	Groundwater flux is a basis for laying out a repository and for calculating nuclide retention.	No indisputable measurement technique exists. Measured discrepancies from predictions may be an artefact of the inability to measure, but also to transform the measured value to a flux in the rock mass. Models generally predict averaged fluxes which is another reason for discrepancy.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
Conductive structures	The appearance and properties of conductive structures are understood (cf. Minor water-bearing zones).	Statistics of frequency and transmissivities were adequately predicted from surface boreholes.	Knowledge of the frequency of conductive structures is basic to DFN-modelling and of importance for repository design.	Assessment based on borehole data, borehole flow metering or packer tests.

	Scientific understanding	**Site-specific knowledge**	**Usefulness**	**Feasibility**
GROUNDWATER CHEMISTRY				
Groundwater mixing	Groundwater mixing is the main process behind the hydrochemical situation at Äspö. Coupling of mixing to a groundwater flow model remains to be done.	Before excavation, four water types were statistically defined. Now a five-component system with five well defined end members has emerged.	The mixing model defines the basic hydrochemistry of the groundwater, which is a basis for performance and safety analyses.	Both sampling and numerical analyses, for the mixing models, can be performed using the technique established by the project.
Groundwater/rock interaction (calcite saturation)	The calcite-carbon dioxide system is rapid. Other groundwater rock interaction systems have not reached equilibrium.	Borehole data, taken before excavation, were basically confirmed.	The calcite-carbon dioxide system defines the pH of the system. This is a basis for performance and safety analyses.	Groundwater sampling and chemical analyses are standard procedures. Sampling for volatile carbon dioxide is difficult.
Ion exchange	The processes of ion exchange with fracture filling materials is basically understood.	Data show substantial ion exchange in historical intrusion of water from different stages of the Baltic sea.	Ion exchange has an influence on the calcite-carbon dioxide system and other solubility limiting solid phases, and retardation of radionuclides.	Groundwater sampling and chemical analyses are standard procedures. The capacity and amount of exchange are difficult to estimate.
Redox reactions	Reducing conditions are expected from a depth of a few tens of metres in any rock formation due to bacterial activity consuming dissolved oxygen in the upper part of the rock, and the reducing capacity of the minerals.	Understanding of how redox conditions develop in the rock has grown considerably during the project.	Redox conditions are essential for performance and safety analyses. At any particular site the understanding needs to be verified by a few observations of high quality.	In-situ measurements of Eh are difficult, but necessary. Stable and feasible relations between Eh and other constituents (e.g. Fe) have been established.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
Biological processes	The original hypothesis was that biological processes exerted insignificant influence on water chemistry.	The knowledge of bacteriology and its influence on water chemistry can still be enhanced. However, it has been demonstrated that they have a great influence on redox sensitive constituents and on concentrations of major constituents. The spatial variability of the process are not well established yet.	Biological reactions influence and sometimes control redox conditions This is of importance for performance and safety analyses.	Methods of taking microbiological samples and analysing the microbiology of the Äspö rock have been developed but need to be further evaluated.

	Scientific understanding	Site-specific knowledge	Usefulness	Feasibility
TRANSPORT OF SOLUTES				
Salinity	The principles behind density-driven flow are established.	The data base supports the interpretations of the salinity models before and during excavation.	Salinity has a significant influence on groundwater flow and transport as well as hydrochemistry and thus influences performance and safety analyses.	Modelling of density-driven flow was developed as a part of the groundwater flow modelling.
Flow paths	Flow paths relate to the connectivity of the rock and are thus coupled to the conductive features. Further understanding of flow and transport phenomena is required.	Three tracer experiments were performed, showing connectivity where hydraulic conductors exist. A preliminary data base on transport properties for non-sorbing species exists.	Reliable models of flow paths and transport times are of great importance for the safety analysis for the repository .	Assessment of transport property data by means other than tracer tests is not evident, other than in a generic sense.
Natural tracers	There is a general understanding of the geological and chemical processes that control the concentrations of natural tracers in relation to time.	The understanding of the evolution of the palaeo-hydrogeological conditions at Äspö was immature at the start of the project. A basic knowledge of the evolution and the distribution of natural tracers has been developed. The data base of the distribution of natural tracers is today reasonably comprehensive.	Natural tracers are important in evaluating and judging the residence time of the groundwater and in interpreting historic and future evolution.	Sampling techniques and tracer analyses are standard procedures. Different isotope methods have been developed during the time since start of the Äspö project.

8.7 EVALUATION OF THE ÄSPÖ RESULTS IN THE CONTEXT OF THE SKB SITING FACTORS

Äspö key issues

Site characterization is a multi- and inter-disciplinary task that necessitates integration during data acquisition, evaluation and presentation of results. In order to facilitate such integration, three basic decisions were made for the site characterization as explained previously. The first was to utilize an iterative approach to the investigations and modelling, the second was to make models to different scales as a means of sorting models used for the Äspö HRL project and the parameter need for each model. The third decision was to divide the site characterization into a set of key issues, namely the *geology*, incorporating the simplified description of lithology and the fracturing, *mechanical stability, groundwater flow, groundwater chemistry* and *transport of solutes.* To each "key issue" a number of ''subjects' were defined that formed the basis for the investigations and the predictions. The main subjects were presented in *Table 8-1.*

The SKB siting factors for the deep repository

On request of the Swedish government in 1993 SKB structured the siting factors into four groups */SKB, 1994/.*

- **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.
- **Land and Environment** - Siting factors of importance for land use and general environmental impact.
- **Societal factors** - Siting factors connected to the development of society and impact on society.

A description of how the siting factors can be applied in the initial siting stage was also provided. One question to be considered for the initial siting stage is:

'A large site with few major fracture zones. This provides extra flexibility in connection with coming investigations and improves the prospects of being able to construct a repository with room for the necessary number of canister positions in sound rock with a high level of safety'

The most important safety-related function of the rock is to safeguard the engineered barriers and, as far as possible, to provide:

- a long-term, stable and suitable chemical environment,

- low groundwater flow
- mechanical stability.

An important safety-related function of the bedrock at a deep repository site is its ability to retain the radionuclides or retard radionuclide transport in the event of a failure of the engineered barriers. The basic requirements on the rock are also, in this case, chemical stability and low groundwater flow.

It is favourable to have recharge area conditions near the deep repository and favourable dilution conditions in the discharge areas, which limit release of radioactive substances to human beings and other living organisms. A basic requirement for modelling of the chemical conditions, the groundwater flow, transport of solutes and the mechanical stability is a good geological-structural model of the site. However, since the basic principle of the SKB deep repository is based on the isolation of the radioactive substances, the factors contributing to isolation are of greater importance than those which are favourable to slow transport in bed rock, sorption and dilution in the far-field.

If possible, sites where future wells and future human intrusion are more probable, for example in ore-bearing bedrock, should be avoided.

The technological siting factors primarily include issues which are of importance for technical feasibility. The underground facility must fulfil the elementary requirements for any underground facility. 'Good rock', i.e. relatively low frequency of fractures and a low hydraulic conductivity of the rock, will facilitate the construction work and is also advantageous from the standpoint of the long-term safety of the repository. Factors which affect the construction work include the rock type, fracture frequency, position and character of the fracture zones, groundwater flow, the size and direction of rock stresses and the mechanical properties of the host rock. It is an advantage if the results of the bedrock investigations can be simply and unambiguously interpreted. This will facilitate the planning and implementation of the investigations, design, performance and safety assessment. No or a very thin soil cover, simple and homogeneous bedrock conditions as well as a regular system of fractures/fracture zones will improve the level of reliability of the prognoses.

Findings of relevance for evaluation of the siting factors

It can first of all be concluded that the "subjects"chosen by the Äspö project are a part of the SKB siting factors developed later.

The Äspö work has given further evidence that the chemistry of groundwater has been stable for long periods of time. The efforts undertaken have also shed more light on the previous history of the groundwater and understanding of the chemical and biological properties that control the composition of the groundwater. Evidence at Äspö have added to previous general knowledge that groundwater at depth is reducing. Further understanding of the biological processes in the rock has taken a major step forward and these findings put even more confidence in the reducing conditions in the rock.

Low groundwater flow is important. The investigations at Äspö show that there is confidence that by appropriate methodology the hydrological properties at a site can be established in a timely manner, even in a complex geological environment, as at Äspö. The findings at Äspö show that near-field models based on pre-investigations should be more reliable in a more homogeneous geological setting.

The question of the long-term mechanical stability is mainly treated within the general SKB Geoscience Programme. The study of mechanical stability at Äspö was mainly devoted to understanding whether mechanical instability will occur during construction and if so, where. The expert judgements on these matters have been correct, which mainly can be attributed to general experience in Sweden that mechanical stability prevails in 'good rock'.

9 CONCLUDING REMARKS

The site investigations for the Äspö Hard Rock Laboratory prior to construction of the facility were planned to meet two requirements. First to conduct the investigations necessary to *design the underground facility* so that it could be constructed with presently available technology without major problems down to a depth of about 500 metres. The construction of the Äspö HRL was made down to a depth of 450 m successfully with only minor layout changes. Secondly to obtain a thorough *understanding* of the rock conditions based on investigations of the surface and investigations in and between boreholes drilled from the surface. The main conclusions concerning the understanding of the rock conditions is summarized below.

Site characterization in conjunction with construction work at Äspö has basically confirmed the pre-construction models. However, the models 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. Standard geological and geophysical methods in combination with hydraulic tests have shown lithological domains and the geometrical framework. Hydraulic tests in and between boreholes have shown the existence of the major hydraulic conductors and their geometry. In spite of scaling problems, reasonable estimates of hydraulic conductivity have been achieved. Sampling of groundwater was done and subsequent chemical analyses have put the Äspö groundwater in a regional context as well as created an understanding of the past evolution of the groundwater at the site. The technology for rock stress measurement and interpretation is available, but additional studies are needed to explain differences in results from different measurements. So far tracer tests have been used to examine the connectivity of the hydraulic framework and to find crude parameter estimates for non-sorbing transport.

Concidering the stage goals the characterization should *demonstrate that investigations at the ground surface and in boreholes provide sufficient data on essential safety-related properties of the rock at repository level (stage goal 1).* The work at Äspö has demonstrated that relevant safety-related data can be obtained. The data set is not complete, but has anyway allowed for safety analyses of a simulated repository at Äspö by the Swedish Nuclear Inspectorate and the SKB (in progress).

The results and experience from Äspö are partly general in nature and partly site-specific 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.

The methods and technology needed for characterization of the rock in the detailed site investigations have been tested and developed (Stage goal 2). Valuable experiences of construction-testing integration have also been obtained. On-going R&D work will supplement present knowledge.

The site characterization at Äspö has been used to *refine and test on a large scale at repository depth methods and models for describing groundwater flow and the transport of solutes in rock (Stage goal 3).* The joint international work in the Äspö Task Force on Modelling of Groundwater flow and Transport of Solutes has demonstrated many different approaches to modelling that seem useful.

Design and construction of the Äspö Hard Rock Laboratory, incorporating both drill-and-blast excavation and mechanical excavation using a tunnel boring machine, has *provided 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 (Stage goal 4).* On-going-experiments at Äspö HRL, such as the planned Prototype Repository will be valuable to transfer general scientific knowledge into engineering practice. For example theoretical development of grouting theory will be useful for the future repository. Valuable work was performed by the project and developments will continue.

Finally, the site characterization at Äspö has been a realistic 'dress-rehearsal' that will be useful for planning and executing surface and underground site characterization for the deep repository for spent fuel in Sweden.

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002a2pw.wpd:	Appendix 2

APPENDIX 1

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APPENDIX 2

GROUNDWATER CHEMISTRY IN FRACTURE ZONES

GROUNDWATER CHEMISTRY IN FRACTURE ZONES

The chemical composition of the groundwater, the saturation index of calcite and carbon dioxide, indication of sulphate reduction, in the different fracture zones (EW-3a, NE-4a,4b, NE-1a,1b, NE2a-1, NE2a-2, NE2a-3, NE-3b,3c, NNW-4H_2O-1, NNW-4H_2O-2,NNW-4H_2O-3) and in the Redox zone over time are listed. In fracture zones with no groundwater sampling boreholes, the boreholes ±100 m from the actual fracture zone were set to represent that fracture zone. If two borehole observations fall inside the range the observation closest to the fracture zone was selected. When the results are interpolated in space (±100 days) the accuracy decreases.

Fracture zone	Representing day (0=90-10-14)	ID code	Penetrating zone	Tunnel length (m)	Date	Inflow rate ($m^3/s*10E^{-3}$)	SNO	Na (mg/L)	K (mg/L)	Ca (mg/L)	Mg (mg/L)	HCO_3 (mg/L)	Cl (mg/L)	SO_4 (mg/L)
Redox zone	150	KR0012B	x	513	91-05-07			352.0	2.0	143.0	15.4	198	695.0	70.0
Redox zone	550	KR0012B	x	513	92-04-22		1940	604.0	4.9	268.0	37.7	245	1330.0	134.4
Redox zone	750	KR0012B	x	513	92-10-28		2026	497.0	5.0	186.0	27.9	292	970.0	176.0
Redox zone	950	KR0012B	x	513	93-05-16		2094	424.0	4.3	136.0	25.1	315	710.0	142.2
Redox zone	1150	KR0012B	x	513	93-11-08		2193	387.0	4.3	118.0	20.4	324	619.0	134.7
Redox zone	1350	KR0012B	x	513	94-08-10		2270	346.6	3.4	100.1	17.4	325	500.0	125.8
NE-4a,4b	350	SA0850B	x	850	91-08-20	0.1-1.2		1920.0	18.0	1210.0	141.0	170	5440.0	90.6
NE-4a,4b	750	SA0813B	x	813	92-12-02	0.1-1.2	2049	1700.0	21.0	364.0	123.0	481	3450.0	186.0
NE-4a,4b	1150	SA0813B	x	813	93-09-29	0.1-1.2	2190	1640.0	19.1	310.0	124.0	317	3350.0	274.5
NE-4a,4b	1350	SA0813B	x	813	94-06-07	0.1-1,2	2253	1578.0	11.9	322.1	121.1	302	3272.3	299.6
NE-3b,3c	350	SA0976B	x	976	91-10-15	3.9		2170.0	20.6	993.0	203.0	500	5590.0	58.8
NE-3b,3c	550	SA1062B		1062	92-04-23	3.9		2230.0	23.5	770.0	220.0	531	5320.0	100.8
NE-3b,3c	750	SA1062B		1062	92-12-02	3.9	2050	1930.0	34.0	545.0	177.0	403	4350.0	189.0
NE-3b,3c	950	SA0958B	x	958	93-06-23	3.9	2121	1829.2	22.4	595.2	137.2	371	4087.9	243.0
NE-3b,3c	1150	SA0958B	x	958	93-09-28	3.9	2181	1810.0	19.6	657.0	144.0	296	4260.0	239.4
NE-3b,3c	1350	SA0958B	x	958	94-06-07	3.9	2254	1634.1	21.4	477.8	125.1	274	3641.0	295.2
NE-1a,1b	550	SA1342B		1342	92-06-16	5.0		1680.0	11.0	950.0	152.0	170	4730.0	148.5
NE-1a,1b	750	HA1327B	x	1327	92-10-15	5.0	2023	1610.0	9.4	648.0	128.0	252	3920.0	225.0
NE-1a,1b	950	SA1229A		1229	93-06-23	5.0	2120	1847.9	24.5	598.5	156.1	426	4210.9	101.0
NE-1a,1b	1150	HA1327B	x	1327	93-12-15	5.0	2208	1760.0	13.7	684.0	157.0	259	4310.0	255.3
NE-1a,1b	1350	SA1229A		1229	94-06-07	5.0	2256	1735.4	26.1	512.1	151.7	336	3928.2	241.5
EW-3a	750	SA1420A	x	1420	92-10-15	0.8	2024	1540.0	10.2	715.0	123.0	170	3930.0	226.2
EW-3a	950	SA1420A	x	1420	93-06-22	0.8	2116	1484.2	9.7	487.9	124.5	215	3419.9	307.0
EW-3a	1150	SA1420A	x	1420	93-09-29	0.8	2183	1600.0	13.7	480.0	139.0	214	3530.0	331.8
EW-3a	1350	SA1420A	x	1420	94-06-07	0.8	2257	1426.5	15.7	395.8	116.8	206	3052.5	290.3
NE-2a-1	750	SA1614B		1614	92-11-19	0.003	2035	1570.0	8.3	1250.0	80.2	37	5160.0	296.4
NE-2a-1	950	SA1614B		1614	93-06-22	0.003	2117	1953.7	5.2	1710.4	65.9	32	6207.3	424.0
NE-2a-1	1150	SA1614B		1614	93-09-28	0.003	2184	1880.0	6.7	1390.0	90.8	81	5650.0	332.4
NE-2a-1	1350	SA1614B		1614	94-06-06	0.003	2249	1831.3	7.4	1207.0	98.3	109	5176.1	322.0
NE-2a-2	750	SA1828B	x	1828	92-11-19	0.003		1700.0	8.5	1290.0	92.2	43	5200.0	303.0
NE-2a-2	950	SA1828B	x	1828	93-06-21	0.003	2115	1909.2	8.0	1392.4	113.9	48	5849.7	362.9
NE-2a-2	1150	SA1828B	x	1828	93-09-28	0.003	2187	1930.0	10.0	1450.0	108.0	48	6010.0	362.7
NE-2a-2	1350	SA1828B	x	1828	94-06-06	0.003	2252	1861.5	11.7	1063.9	138.8	111	5123.0	259.9
NE-2a-3	1150	SA2583A		2583	94-03-07	0.003	2223	2099.0	8.3	1870.0	56.9	13	6647.0	462.0
NE-2a-3	1350	SA2583A		2583	94-05-18	0.003	2240	2170.0	8.5	1859.6	73.9	44	6895.6	442.6
NNW-4H_2O-1	950	SA2074A		2074	93-06-17	0.06-0.12	2113	1959.4	8.6	992.6	172.0	47	5282.5	299.0
NNW-4H_2O-1	1150	SA2074A		2074	93-09-28	0.06-0.12	2173	1730.0	11.0	764.0	144.0	79	4670.0	263.1
NNW-4H_2O-1	1350	SA2074A		2074	94-06-07	0.06-0.12	2258	1701.7	10.2	723.2	141.5	94	4275.6	270.9
NNW-4H_2O-2	950	SA2109B	x	2109	93-02-15	0.06-0.12		1730.0	17.0	884.0	107.0	67	4480.0	303.0
NNW-4H_2O-2	1150	SA2142A		2142	93-12-02	0.06-0.12	2202	1720.0	25.0	581.0	128.0	127	3880.0	367.8
NNW-4H_2O-2	1350	SA2175B		2175	94-05-30	0.06-0.12	2244	1959.5	15.3	1037.1	161.6	127	5442.0	261.6
NNW-4H_2O-3	1350	KA3191F		3191	94-06-04	0.06-0.12	2248	2225.3	8.6	2093.1	64.3	29	7409.7	445.2

Fracture zone	Representing day (0=90-10-14)	ID code	^3H (TU)	^2H (SMOW)	^{18}O (SMOW)	Fe(tot) (mg/L)	Fe^{2+} (mg/L)	DOC (mg/L)	pH (units)	Calcite (log IAP/KT)	Log pCO_2 (bar)	Indicator of sulphat reduction
Redox zone	150	KR0012B	34.0	-82.1	-11.4	0.200	0.200		7.8	0.49	-2.62	
Redox zone	550	KR0012B	25.0	-77.3	-10.2	0.287	0.291	12.0	7.7	0.66	-2.46	
Redox zone	750	KR0012B	17.0	-79.9	-9.9	0.218	0.216	14.0	7.7	0.60	-2.37	
Redox zone	950	KR0012B	17.0	-72.0	-9.9	0.186		18.0	7.5	0.32	-2.14	
Redox zone	1150	KR0012B	34.0	-69.6	-9.6	0.179		11.3	7.4	0.18	-2.03	
Redox zone	1350	KR0012B	31.3	-68.1	-9.8	0.189			7.3	0.02	-1.93	
NE-4a,4b	350	SA0850B	6.8	-67.2	-8.3				7.7	0.93	-2.70	
NE-4a,4b	750	SA0813B	6.8	-59.8	-7.5	6.330	6.330	8.3	7.3	0.53	-1.82	Bacteria
NE-4a,4b	1150	SA0813B	14.0	-50.4	-7.3				7.1	0.07	-1.82	
NE-4a,4b	1350	SA0813B	28.7	-53.7	-7.2				7.0	-0.05	-1.75	
NE-3b,3c	350	SA0976B	14.0	-60.4	-7.4				7.2	0.79	-1.75	GW
NE-3b,3c	550	SA1062B	8.0	-58.0	-7.7			11.0	7.3	0.83	-1.81	GW
NE-3b,3c	750	SA1062B	9.3	-57.6	-7.3	2.160	2.160	9.1	7.3	0.59	-1.91	Bacteria
NE-3b,3c	950	SA0958B	8.4	-56.0	-7.5	3.334	3.323		7.0	0.27	-1.68	
NE-3b,3c	1150	SA0958B	14.0	-57.5	-7.4				7.5	0.75	-2.24	
NE-3b,3c	1350	SA0958B	28.7	-55.6	-7.2				7.0	0.06	-1.80	
NE-1a,1b	550	SA1342B	5.9	-61.9	-8.7				7.3	0.44	-2.30	
NE-1a,1b	750	HA1327B	17.0	-65.3	-7.4	2.160	2.150		7.4	0.58	-2.21	Bacteria
NE-1a,1b	950	SA1229A	16.0	-60.0	-7.3	2.891		21.0	7.0	0.33	-1.62	GW
NE-1a,1b	1150	HA1327B	18.0	-50.6	-7.5	2.640	2.430	4.8	6.9	0.05	-1.76	
NE-1a,1b	1350	SA1229A	22.0	-52.8	-7.0				7.0	0.17	-1.72	
EW-3a	750	SA1420A	17.0	-72.0	-8.7	1.110	1.110		7.6	0.66	-2.57	
EW-3a	950	SA1420A	31.0	-59.0	-7.5	1.941	1.920		7.3	0.30	-2.18	
EW-3a	1150	SA1420A	22.0	-52.5	-7.0				7.3	0.29	-2.18	
EW-3a	1350	SA1420A	33.8	-57.0	-7.5				7.2	0.10	-2.10	
NE-2a-1	750	SA1614B	8.0	-103.1	-13.1			1.0	7.4	-0.01	-3.06	
NE-2a-1	950	SA1614B	4.2	-85.5	-11.5	0.309	0.298	1.0	7.6	0.22	-3.34	
NE-2a-1	1150	SA1614B	4.2	-77.6	-10.4			1.0	7.4	0.35	-2.73	
NE-2a-1	1350	SA1614B	8.4	-71.9	-9.7				7.2	0.22	-2.41	
NE-2a-2	750	SA1828B	4.2	-84.4	-10.8				7.4	0.06	-3.00	
NE-2a-2	950	SA1828B	4.2	-75.9	-10.3	0.865	0.848	1.0	7.4	0.12	-2.96	
NE-2a-2	1150	SA1828B	4.2	-71.4	-10.3			1.0	7.3	0.03	-2.87	
NE-2a-2	1350	SA1828B	8.4	-67.8	-8.9				7.2	0.18	-2.40	
NE-2a-3	1150	SA2583A	4.2	-85.9	-10.7	0.242	0.236	0.4	7.5	-0.25	-3.64	
NE-2a-3	1350	SA2583A	5.9	-83.5	-11.1	0.373			7.9	0.67	-3.51	
NNW-4H_2O-1	950	SA2074A	5.9	-65.2	-8.5	0.755	0.734	1.0	7.0	-0.45	-2.60	
NNW-4H_2O-1	1150	SA2074A	7.0	-60.0	-8.4			1.0	7.1	-0.20	-2.45	
NNW-4H_2O-1	1350	SA2074A	10.1	-63.3	-8.5				7.3	0.08	-2.55	
NNW-4H_2O-2	950	SA2109B	5.9	-64.5	-8.2				8.1	0.82	-3.49	
NNW-4H_2O-2	1150	SA2142A	21.0	-56.2	-7.2	0.881		3.4	7.4	0.23	-2.50	
NNW-4H_2O-2	1350	SA2175B	8.4	-62.0	-8.2	0.882			7.8	0.84	-2.92	
NNW-4H_2O-3	1350	KA3191F	8.4	-81.6	-11.2				7.3	-0.08	-3.11	

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