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## Site descriptive modelling
## Äspö SDM

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# Abstract

The groundwater data from the Äspö local area including the Äspö Hard Rock Laboratory (Äspö HRL) constitute unique material due to the number of samples, the duration of the sampling period, the often extensive analytical scheme (or analytical programme), the generally good quality of the data and the amount of supportive data from other geoscientific disciplines resulting from the pre-investigation, the excavation of the tunnel, and from subsequent operation of the facility. However, due to the complex hydraulic situation and the varying nature of the data, a clear organisation and evaluation of the data is of paramount importance prior to interpretation and modelling.

The hydrochemical data, representing a total of 3,180 groundwater samples collected and analysed during the time period 1986 to 2011, have been evaluated with respect to their usefulness for modelling purposes using basically the same approach as for the SFR extension data (Nilsson et al. 2011) and the PLU data (Smellie et al. 2008, Smellie and Tullborg 2009, Laaksoharju et al. 2008, 2009).

The major concerns have been:

- To facilitate future interpretation and modelling work by the organisation of well structured data tables representing quality categorised data.
- To give a detailed and well supported description of the data.
- To identify samples that may have been affected by the experimental conditions and are unsuitable for general modelling purposes. Samples collected during different projects may represent sampling conditions that are not comparable to the regular sampling situation. For example, sampling from a circulating water system connected to the sampled borehole section, or from a borehole into which water has been injected.
- To identify other unsuitable samples, for example incomplete analyses, impact from grouting, high charge imbalance indicating unacceptable analytical performance etc.
- To identify samples that may be used for special purposes in additional datasets but otherwise unsuitable for regular modelling work, and to guide the future user in how best to use data from these special datasets.

The data evaluation has resulted in a well structured dataset containing quality categorised data of high quality for general interpretation and modelling purposes (1,585 samples in Dataset I), a minor dataset with rejected data (674 samples in Dataset II), and a few additional subdatasets containing data that may be used with caution for other special purposes. The data evaluation and the derived datasets are described in this report.

# Sammanfattning

Insamlade grundvattendata från Äspö området inklusive Äspölaboratoriet (Äspö HRL) utgör ett unikt material på grund av det stora antalet prov och provtagningsperiodens längd, det omfattande analysprogrammet, god datakvalitet, och mängden understödjande data inom andra geovetenskapliga discipliner från förundersökningen, byggfasen och från driften av anläggningen. Den komplexa hydrauliska situationen och varierande beskaffenhet hos data gör dock att det är nödvändigt med en förberedande organisation och utvärdering av datamängden innan data kan användas för tolkning och modellering.

Därför har hydrokemiska data motsvarande totalt 3 180 grundvattenprov som insamlats under tidsperioden 1986 till 2011 utvärderats med avseende på användbarhet för modellerings- och tolkningsändamål med hjälp av i stort sett samma metodik som inom projektet SFR-utbyggnad (Nilsson et al. 2011) och inom platsundersökningarna i Forsmark och Oskarshamn (Smellie et al. 2008, Smellie and Tullborg 2009, Laaksoharju et al. 2008, 2009).

Den huvudsakliga inriktningen har varit;

- Att underlätta framtida tolknings- och modelleringsarbete genom att organisera välstrukturerade datatabeller med data kategoriserade med avseende på provkvalitet.
- Att ge en detaljerad och väl underbyggd beskrivning av data/prov-mängden.
- Att identifiera prov som kan ha påverkats av experimentella förhållanden från datasetet avsett för modelleringsändamål. Prov som har tagits ut inom olika projekt kan representera provtagningsförhållanden som inte är jämförbara med den normala provtagningssituationen, till exempel prov tagna från ett cirkulerande system kopplat till en borrhålssektion eller från ett borrhål där vatten har injekterats.
- Att identifiera andra olämpliga prov: orsaken kan vara ofullständiga analyser, påverkan av injekteringsbruk, stort fel i jonbalansen som indikerar oacceptabla analyser etc.
- Att identifiera prov som kan användas för speciella ändamål och studier i speciella dataset även om de är olämpliga för normalt modelleringsarbete och att guida framtida användare av data i hur dessa andra dataset kan användas.

Datautvärderingen har resulterat i ett välstrukturerat dataset (1 585 prov i Dataset I) som innehåller kvalitetskategoriserade prov med data av hög kvalitet för tolknings och modelleringsarbete, ett mindre dataset med förkastade data (674 prov i Dataset II) och några övriga dataset med data som kan användas med viss försiktighet för andra speciella ändamål. Datautvärderingen och dataseten beskrivs i denna rapport.

# Contents

# 1 Introduction

## 1.1 Background

The Swedish Nuclear Fuel and Waste Management Company (SKB) established the Äspö Hard Rock Laboratory (HRL) in the early 1990s in order to serve as a test area for SKB's work to design and construct a deep geological repository for spent nuclear fuel. The purpose was also to develop and test methods to describe and evaluate future candidate sites for a deep repository.

Considerable amounts of geoscientific data have been produced at the Äspö HRL derived from different investigations and disciplines (geology, geophysics, rock mechanics, hydrogeology, hydrochemistry etc) since the start of the pre-investigations in 1986. The investigation work can be divided into three phases focused on different major/main tasks as listed below:

- *Pre-investigation phase from 1986 to 1990.* Studies were performed to provide the necessary information to decide the location of the HRL; this phase also included planning for the construction and operation phases. Furthermore, the geological, hydrogeological and geochemical conditions in the target bedrock volume were predicted from the investigation results in order to allow comparison with subsequent observations during the construction phase and the excavation of the HRL (Smellie and Laaksoharju 1992).
- *Construction phase from 1990 to February 1995.* Comprehensive investigations and experiments were performed in parallel with the construction of the laboratory, i.e. excavation of the main access tunnel to a depth of 450 m and creation of the Äspö Research Village. At the conclusion of the construction stage, different models were compiled and evaluated as a first attempt to establish a multidisciplinary site descriptive model. This resulted in a series of technical reports such as Stanfors et al. (1997a, b) and Rhén et al. (1997a, b, c).
- *Operation phase, ongoing since 1995.* Different experiments and studies have been and are being performed in the Äspö HRL; a summary is given in Chapter 2. A previous modelling exercise (GeoMod) updated the existing hydrogeochemical model by integrating new data covering the operation period 1995–2002 (Laaksoharju and Gurban 2003). Numerous data have been produced since then and therefore it should be possible to update the site descriptive model of Äspö.

In order to facilitate possible future modelling at Äspö, prior organisation and evaluation of all the hydrochemical data is a compulsory pre-requisite, and that is the main aim of this report. There are several important circumstances that make this preparatory work necessary: 1) the Äspö hydrochemical dataset includes data that cover a long time period from 1988 to the present, 2) the groundwater samples collected and analysed, belong to many different projects and, therefore, they were taken for very different purposes, 3) the sampling techniques as well as the analytical protocol and methods have changed with time thus influencing the quality and variability of the analytical data, 4) the number of samples collected from each borehole and borehole section differs considerably; this, and the sporadic sampling complicates the evaluation of groundwater changes and trends, and 5) investigation activities (some of them implying discharge of large volumes of groundwater), as well as occasional drilling and construction work, have frequently occurred over time and might have impacted on the samples.

Together with this, the Äspö hydrogeochemical dataset represents an artificially imposed dynamic flow system with the addition of other anthropogenic effects to the normal gradual changes caused by the presence of the tunnel system, i.e. similar situation to the SFR extension investigations (SKB 2011, Nilsson et al. 2011). This complex situation underlines the importance of conducting a thorough data evaluation and a well organised data selection procedure for future modelling work.

## 1.2 Objectives and report layout

The main aim of the work presented in this report is to systematically describe and evaluate the existing hydrogeochemical data considering the complex situation of the system itself (with all the anthropogenic effects added to the normal evolution of the site), and the nature of the data (with very different qualities and uses). These data will constitute the basis for future interpretation and modelling work to understand the hydrogeochemical conditions at the site.

The report has been structured as follows. After the introduction presented in this first chapter, Chapter 2 addresses the different projects in the Äspö HRL; the performed investigations and the impact on sampling and sampling conditions from different sources such as grouting, drilling/drilling water, sampling techniques, hydrogeology and other forms of contamination. The available hydrogeochemical data, including also colloids, microbes, gasses, porewaters and fracture minerals, are presented in Chapter 3. Chapter 4 presents the criteria used for the sample quality assessment and describes the categorisation process. Chapter 5 presents the results of the categorisation for the whole hydrochemical data set. Chapter 6 describes in detail the different object types (boreholes/borehole sections) and the category of the samples taken from them. Chapter 7 presents the final selection of data to be used for different purposes in any continuing interpretation and modelling work. Finally, as a sort of conclusions, Chapter 8 presents the experiences and lessons learnt from this work.

There are four appendices with additional information. Appendix 1 compiles the information on detection/reporting limits and measurement uncertainties. Appendix 2 reports the corrections made on data concerning some section limits. Appendix 3 presents plots with available Eh and pH logs. Finally, Appendix 4 presents the data from the ongoing Äspö extension project; these data are treated separately to facilitate inclusion of any additional data that will be produced during the writing of this report.

## 1.3 Shortcomings or factors that were not considered in the evaluation work

Only a minor part of the large amount of reports produced during the different investigation phases have been studied (see reference list). This is due to time and cost constraints and therefore it is possible that important information for the data quality assessment may have been overlooked. The information in reports is especially essential for data that were produced a long time ago when the procedures and routines used may now be irrelevant or invalid. It is strongly recommended to check the documentation before starting using the data, mainly in cases such as Data Set IV (experiments). Assuming the limitations with respect to this point, the strategy has been to exclude rather than include data in Dataset I (for normal modelling purposes).

Moreover, the integration with the other disciplines has been very limited. The data evaluation and the production of the data report within the hydrogeochemistry discipline have been ahead of the evaluation work carried out within the other disciplines. Therefore, possible correlation between geological entities and groundwater composition has not been studied and the hydraulic situation in the different sampled borehole sections and its implication for sample quality has not been considered. For example, pressure responses between borehole sections and sudden pressure disturbances in the monitored borehole sections should, ideally, be evaluated and integrated with the hydrogeochemical data. Furthermore, to study the hydraulic transmissivities, the position and the number of the different flow anomalies in the sampled borehole sections is important to ascertain the possibility to collect representative samples from the bedrock formation without the time consuming discharge of large volumes of water.

Finally, the aims and ambitions of this exercise have changed since the hydrogeochemical data evaluation work started. Initially, this report was meant to be the first report of two, the second being the hydrogeochemical site descriptive model for the Äspö site (Äspö SDM). The modelling work was also thought to provide the opportunity to test modelling methods and strategies within the Detum project (Detailed investigation methods). These future modelling plans are, however, uncertain at the completion date of this report. Furthermore, another aim was to evaluate and model the data in parallel with the progress of the ongoing Äspö extension project. However, as this is a data report and the groundwater data will be updated and reported in a regular basis elsewhere, the project has only been briefly discussed in Appendix 5.

## 1.4 Nomenclature and abbreviations

### 1.4.1 Idcode or borehole name convention

All sampled objects (boreholes, weirs, water-yielding fractures on a rock wall surface etc) have idcodes according to a fixed name convention as follows:

**Idcodes for surface boreholes**

- The first letter in a borehole name 'K' or 'H' denotes core drilled and percussion drilled boreholes respectively (in Swedish: Kärnborrhål and Hammarborrhål).
- The two next letters 'AS', 'AV', 'SH', 'LX' and 'BH' stands for Äspö, Ävrö, Simpevarp, Laxemar and Bockholmen respectively; see Figure 3-1.
- The following number (ex. KAS02) is the number of the borehole.

**Idcodes in the HRL**

The object idcode is represented by TDLLLLP where T=type of object and D is tunnel designation, LLLL is the position according to the tunnel section chainage in metres, and P is the position in the tunnel as explained in Figure 1-1.

| T | Object alternatives | D | Tunnel description |
|---|---|---|---|
| P | Geological mapping surface or sampled surface leakage point (initially Y) on roof or walls in tunnels | A | Main tunnel |
| | | F | Side tunnel F |
| K | Core drilled borehole | G | Side tunnel G |
| S | Probing borehole | I | Side tunnel I |
| M | Measurement weir | J | Side tunnel J |
| T | Tunnel (S within an idcode means Side tunnel) | M | Method tunnel |
| | | P | Äspö extension side tunnel P |
| | | R | Redox tunnel |
| | | U | Äspö extension side tunnel U |
| | | X | Side tunnel X |
| | | Z | Zedex side tunnel |

* Redox and Zedex relates to short tunnels or niches excavated for specific experiments (e.g. Large Scale Redox and ZEDEX experiments).

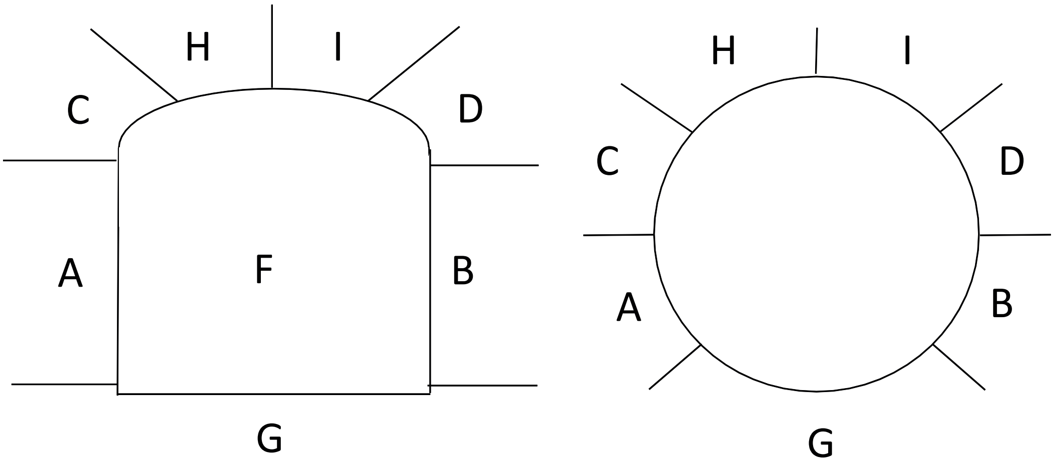

*Figure 1-1. Denotation of different positions on the tunnel wall (drill and blast tunnel and TBM tunnel (modified from Almén and Stenberg 2005).*

**Some examples:**

| | |
|---|---|
| HAS02 | The second percussion borehole drilled from the surface at Äspö. |
| KA0644B | Core drilled borehole in tunnel A, located 644 m along the tunnel on the right side. |
| HA1272A | Percussion borehole in tunnel A, located 1,272 m along the tunnel on the left side. |
| MA1033G | Measurement weir in tunnel A, located 1,033 m along the tunnel at floor level. |
| TASZ | Tunnel name meaning "Side tunnel Z from main tunnel A" (old idcode before 1996 was TZ). |

Exceptions from the convention given above exist especially for boreholes drilled for special projects. For example boreholes KXBLOTS1 (pilot hole no 1) and KXBLOTA1 (pilot hole no 2), where K stands for core drilled hole, X for experiment, B for bentonite/buffer type of experiment, LOT for the experimental series, A for adverse test conditions and S for standard conditions, and finally 1 for the first experiment of the type.

### 1.4.2 Explanation of terms, symbols, subscripts and abbreviations

Terms, symbols, subscripts and abbreviations that occur in the report are explained in Table 1-1.

**Table 1-1. Terms, symbols, subscripts and abbreviations used in this report**

| Symbol/abbreviation | Description |
|---|---|
| AA | Autotrophous Acetogens. |
| AAS | Atomic Absorption Spectrometry. |
| AM | Autotrophous Metanogens. |
| AMS | Accelerator Mass Spectrometry. |
| AS | Alfa spectroscopy. |
| ATP | AdenosineTriPhosphate. |
| BIPS | Borehole Image Processing System. |
| CCC | Complete Chemical Characterisation. |
| CDT | Cañon Diablo Troilite (standard used for $\delta^{34}S$). |
| CHAB | Cultivable Heterotrophic Aerobic Bacteria. |
| Dilution test | Test implying addition of concentrated tracer to a borehole section and measurment of the dilution in order to determine natural groundwater flow. |
| EC | Electrical Conductivity. |
| End member | Original water (e.g. Glacial melt-water, meteoric water, Littorina water etc) contributing to groundwater mixture. |
| Filtering on line | The filtering is performed with the filter holder connected directly to the outlet tubing from the borehole section and the filtrate is collected in the sample bottle. |
| Formation groundwater | Groundwater originating directly from fracture systems in the bedrock in contrast to *section water;* see below. |
| GWCM | Groundwater Chemical Monitoring (long term regular sampling). |
| HA | Heterotrophous Acetogens. |
| HM | Heterotrophous Metanogens. |
| HMS | Hydro Measurement System (system for regular pressure measurements in isolated borehole sections). |
| HRL | Hard Rock Laboratory (e.g. Äspö HRL). |
| HTHB | Hydraulic test equipment for percussion boreholes. |
| ICP AES | Inductively Coupled Plasma Atomic Emission Spectrometry. |
| ICP MS | Inductively Coupled Plasma Mass Spectrometry. |
| ICV | Input 'Compositional Variables' in M3 mixing calculations. |
| Idcode | Name of sampling location or other investigated object in the Sicada database. |
| INAA | Instrumental Neutron Activation Analyses. |
| Injection test | Test to determine of the hydraulic transmissivity, here in 3 m or 30 m intervals. |
| IRB | Iron Redducing Bacteria. |

| Symbol/abbreviation | Description |
|---|---|
| LIBD | Laser Induced Breakdown Detection. |
| LSC | Liquid Scintillation Counting. |
| LTD | Long Term Diffusion experiment. |
| M3 | Computer software for mixing calculations. |
| M.a.s.l. | Metres above sea level. Coordinate system RT90- RHB 70. |
| Mbl | Metre borehole length (length measured from top of casing, the zero point, along the borehole). |
| Measurements *in situ* | Measurements performed in flow through cell located within the borehole and within or connected adjacent to the investigated borehole section. |
| Measurements on-line | Measurements performed in flow through cell connected directly to the outlet tubing from the investigated borehole section. |
| MOB | *Methane-Oxidizing Bacteria.* |
| MRB | Manganese Reducing Bacteria. |
| MS | Mass Spectrometry. |
| NRB | Nitrogen Reducing Bacteria. |
| PEEK | Polyether Ether Ketone. |
| PDB | *Pee Dee Belemnite.* |
| PFL logging | Flow logging using Posiva Flow Log equipment. |
| PFL-f | Descrete inflow detected by the Posiva flow logging method. |
| PLU | Site investigation projects carried out in Forsmark and Oskarshamn (2002–2007) to select locations for the planned repository for radioactive waste. |
| pmC | Percent of modern Carbon. |
| Probing borehole | Regularly drilled approx. 20 m long boreholes along the HRL tunnels; see Section 6.2. |
| Quality assurance | The concept of quality assurance as it is applied in this report implies checking the data import to the Sicada database so that the stored values agree with the values reported by the laboratories, as well as initial simple consistency checks and plausibility judgements. The records are then marked with QC. The data may not be exported until this has been done. |
| REES | Rare Earth Elements. |
| REX | Redox Experiment in Detailed Scale. |
| RHB 70 | An improvement of the elevation reference system RH 70. |
| RNR | RadioNuclide Retention experiment. |
| Sample series | Several separate sampling occasions (annually, every fifth year or weeks to months in between the main occasions). |
| Sampling *in situ* | The sample is enclosed in the investigated borehole section and transferred to the ground surface at maintained pressure. |
| Section water | Groundwater that has been stagnant in the borehole for some time. Its composition may be different from formation groundwater; especially the sulphide concentration may have changed/increased. |
| SGU | The Swedish Geological Survey (Sveriges Geologiska Undersökningar). |
| Sicada | SKBs database for primary data. (Site Characterisation Database). |
| SRB | Sulphate Reducing Bacteria. |
| SS | Swedish Standard method. |
| Surface boreholes | Boreholes drilled from the surface. |
| TASA | Tunnel A, the main tunnel. |
| TASU | Tunnel U, from the main tunnel A. |
| TASP | Tunnel P, from the main tunnel A. |
| TDS | Total Dissolved Salts/Solids. |
| Time series | At least three samples collected during continuous pumping or discharge from a tunnel borehole (duration of days or weeks). |
| TIMS | Thermal Ionisation Mass Spectrometry. |
| TRUE | Tracer Retention Understanding Experiment. |
| Tunnel boreholes | Boreholes drilled from the tunnel. |
| Weir | In this report, embankment or dam for measuring inflowing water to a specific tunnel interval (water sampling object type), see Section 6.5. |
| V-SMOW | Standard Mean Ocean Water (standard used for $\delta^{18}O$). |

# 2 Investigations and investigation prerequisites

Large amounts of data have been produced representing very different objectives during more than 25 years of pre-investigations, construction and operation, and data are still being produced in different ongoing research projects. This chapter briefly describes the different investigation phases with focus on investigations and projects involving groundwater sampling or of relevance for the evaluation of groundwater sample representativity.

The last part of the chapter treats possible impacts from the presence of the tunnel system as well as from other activities that might influence the sampling and sampling conditions. Even assuming that every means have been taken to try and avoid possible contamination or modification, the system has been inherently altered and this must be taken into account when interpreting the final results.

## 2.1 Pre-investigation phase

The pre-investigation phase at Äspö (1986–1990) can be divided into three stages, the sitting stage, the site description stage and the prediction stage (Almén and Zellman 1991). During the pre-investigations, a new core drilling technique was used, telescope-type drilling, which allowed contemporary airlift pumping to minimise contamination by drilling debris or flushing water.

Investigations during the *siting stage* were performed in order to obtain a first indication of site suitability for an underground facility and the best place for its location. The studies were mainly based on airborne geophysics and investigations from the ground surface. However, 23 percussion boreholes were drilled during 1987 and included twelve boreholes in Äspö, (HAS01 to 12) seven boreholes in Laxemar (HLX01 to 07) and four boreholes in Ävrö (HAV01 to 04). Groundwater sampling in the boreholes was conducted immediately after the boreholes were drilled using light portable pump-single packer equipment in order to provide background information on the composition of shallow groundwaters (Almén and Zellman 1991). Table 2-1 below shows which borehole investigations were performed in the different percussion boreholes drilled at this stage. Lineaments were interpreted from digital terrain models and fracture mapping and special tectonic studies were also performed. Furthermore, analyses were made of data from the SGU Well Records and of hydrogeological data from the pre-investigation and construction works for the power plant and the Clab interim storage facility for spent nuclear fuel. The goal was to describe the main fracture systems and the main sets of tectonic zones and to define the shallow groundwaters in the area. Based on data from this first stage, the Äspö area was selected as a preferential site for the HRL and a first conceptual model was subsequently developed (Gustafsson et al. 1991).

The *site description stage* included extensive geoscientific investigations. The core drilling programme (1988–1989) included three boreholes on Äspö (KAS02, 03 and 04) and one reference borehole on Laxemar (KLX01). The boreholes were located based on a preliminary geological model and the purpose was to investigate major structures. Detailed hydrogeochemical investigations were performed in water yielding borehole sections in cored boreholes using the mobile chemistry units for advanced groundwater sampling. Table 2-2 below shows the type of borehole investigations performed in the different cored boreholes drilled at this stage.

The *prediction stage,* following selection of the southern part of Äspö as the most suitable location for the HRL, implied detailed characterisation of this part of the island and the aim was also to predict how an underground construction will influence the hydraulic behaviour of the rock volume. Four additional cored boreholes (KAS05, 06, 07 and 08) and five percussion boreholes (HAS13, 14, 15, 16 and 17) were drilled. The cored boreholes were drilled down to a vertical depth of 500 m and all were directed towards indicated zones of geological and hydrogeological importance. A complementary drilling programme, which included boreholes KAS09, 10, 11 and 14 and KBH02, was conducted after the decision was made to locate the entrance to the tunnel at Simpevarp. These boreholes were drilled to localise and characterise fracture zones in the tunnel area (mainly to obtain more information on the fracture zones EW-1 and NE-2 south of Äspö). Borehole KBH02 was drilled almost horizontal from Hålö-Äspö and approximately parallel to the planned tunnel direction. Additional boreholes (KAS12 and 13 as well as the percussion boreholes HAS18, 19 and 20) were drilled to obtain further information of the fracture zones on southern Äspö. Groundwater sampling was performed in most of the cored boreholes but not in the percussion boreholes. However, groundwater samples were collected during 2005 from some of these later percussion boreholes.

**Table 2-1. Tests/investigations in the different percussion drilled boreholes during the pre-investigation phase and boreholes that have been later sampled[4]; modified from Almén and Zellman (1991).**

| | Percussion drilled boreholes HAS01–HAS20 | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 01 | 02 | 03 | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| **Length (m) / Dip (°)** | 100 / 61 | 93 / 55 | 100 / 56 | 200 / 61 | 100 / 58 | 100 / 88 | 100 / 62 | 125 / 58 | 125 / 59 | 125 / 61 | 125 / 89 | 125 / 60 | 100 / 63 | 100 / 88 | 120 / 60 | 120 / 60 | 120 / 60 | 150 / 62 | 150 / 57 | 150 / 60 |
| **Drilling data[1]** | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X |
| **Geophysical logging[2]** | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X |
| **Hydrogeology** | | | | | | | | | | | | | | | | | | | | |
| Airlift test, intervals | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X | X |
| Injection test, 3 m interval[5] | | | | | | | | | | | | | | | | | | | | |
| Injection test, 30 m interval[5] | | | | | | | | | | | | | | | | | | | | |
| Spinner (flow meter logging) | | | | | | | | | | | | | | | | | | | | |
| Pumping test[5] | | X | X | | X | | X | | | | | | | | | | | | X | |
| Pumping interference test[5] | | | | | | | | | | | | | X | | | | | | | X |
| Dilution test, intervals[5] | | | | | | | | | | | | | | | | | | | | |
| Observation, packer settings | | | | | | | | | | | | | | | | | | | | |
| Fluid conductivity | | | | | | | | | | | | | | | | | | | | |
| Installed circulation sections | | | | | | | | | | | | | | | | | | | | |
| **Groundwater chemistry** | | | | | | | | | | | | | | | | | | | | |
| Complete chemical characterisation | | | | | | | | | | | | | X | | | | | | | |
| Sampling during drilling | | | | | | | | | | | | | | | | | | | | |
| Sampling campaign using simple packer equipment[3] | | X | X | | X | X | X | | | | | | | | | | | | | |
| Monitoring programme[4] | | | | | | | | | O | | | | | O | | | | O | O | |

[1] Includes core logging and petrophysics.

[2] Includes borehole deviation, calliper + magnetic suscept, sonic, natural gamma, density + neutron, resistivity + spontaneous potent, temperature, borehole fluid resistivity and radar.

[3] Documented in Almén and Zellman (1991).

[4] O means sampling programme following the pre-investigation phase.

[5] The method is explained in Table 1-1.

**Table 2-2. Tests/investigations in the different core drilled boreholes during the pre-investigation phase and boreholes included in subsequent monitoring programmes; modified from Almén and Zellman (1991).**

| Boreholes | Cored boreholes KAS02–KAS14 | | | | | | | | | | | | | KBH02 | KLX01 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 02 | 03 | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 | 12 | 13 | 14 | | |
| Length (m) / Dip (°) | 924 / 85 | 1002 / 85 | 481 / 60 | 550 / 85 | 602 / 60 | 604 / 59 | 601 / 60 | 450 / 60 | 99 / 60 | 249 / 89 | 380 / 69 | 406 / 62 | 212 / 60 | 706 / 45 | 702 / 85 |
| **Core loggin$^{G}$** | X | X | X | X | X | X | X | X | | X | X | X | X | X | X |
| **Petrophysics** | X | | | | | | | | | | | | | | X |
| **Geophysical logging** | X | X | X | X | X | X | X | X | | X | X | X | X | | X |
| **Rock stress measurements** | X | X | X | | | | | | | | | | | | |
| **Hydrogeolog$^{Y}$** | | | | | | | | | | | | | | | |
| Airlift test, interva$^{ls}$ | X | X | X | X | X | X | X | X | | X | X | X | X | X | X |
| Injection test, 3 m interval | X | X | X | X | X | X | X | | | | | | | | X |
| Injection test, 30 m interval | X | X | | | | | | | | | | | | | X |
| Spinner (flow meter logging$^{)}$ | X | X | X | | X | X | X | X | | X | X | X | X | | |
| Pumping tes$^{t}$ | X | X | X | X | X | X | X | X | | | | | X | | X |
| Pumping interference test | X | X | | | X | X | | X | | X | X | X | X | X | |
| Dilution test, intervals | X | X | X | X | X | X | X | X | | X | X | X | X | X | |
| Observation, packer settings | X | X | X | X | X | X | X | X | | X | X | X | X | X | |
| Fluid conductivity | X | X | X | X | X | X | X | X | | X | X | X | X | X | |
| Installed circulation sections | X | X | X | X | X | X | X | X | | X | X | X | X | X | |
| **Groundwater chemistry** | | | | | | | | | | | | | | | |
| Complete chemical characterisation | X | X | X | | | | | | | | | | | | X |
| Sampling during pumping test | X | X | | | X | | | | | | | | | | |
| Sampling during drilling | | | | X | X | X | X | X | | X | X | X | X | X | X |
| Fracture mineral analyses and statistics | X | X | X | X | X | X | X | | | | | | | | X |
| Fracture mineral chemistr$^{y}$ | X | | | | X | | | | | | | | | | X |
| Monitoring programme$^{*}$ | O | O | O | O | O | O | O | O | | O | O | | O | | |

* See explanations below Table 2-1.

## 2.2 Investigations performed during tunnel excavation

During the construction of the Äspö HRL, follow-up and documentation work were carried out to collect sufficient geological, rock mechanical, hydrogeological and hydrogeochemical data to validate the predictions made on the basis of the pre-investigations. The underground documentation work comprised:

- One hour documentation at the tunnel face, roof and walls (last round) including basic mapping of rock types, fractures, fracture filling material, other structures, water inflows and photographing. The available time was restricted to avoid delays in the construction work.
- Water samples were collected at leakage points in the tunnel face, roof and walls. Restricted sampling in the area of the final blasting round was carried out at a few points where the flow exceeded 1 litre/min. Smaller leaks were sampled further from the tunnel front without any time restrictions.
- Documentation during and after the drilling of probing holes was conducted with the aim of (1) documenting the rock quality and conditions in the four subsequent rounds and in the immediate surroundings of the tunnel, (2) observing the occurrence of water ahead of the working face by measuring flow and pressure, and (3) obtaining pressure observations over a longer period of time in isolated borehole sections.

- Documentation of 50 m rock blocks to provide complementary data collected to improve the data coverage in the 50-m blocks and validate the previous predictions (for predictions prior to excavation and the process of their validation, see Gustafsson et al. (1991)).
- Flow observations.

Besides the probing boreholes (see explanation in Table 1-1), both percussion and cored boreholes were drilled for special studies (often from side tunnels) that were performed during the construction phase. Some of these special studies included groundwater sampling and analyses and furthermore some of the boreholes drilled for these studies have been sampled subsequently for groundwater analyses as part of the regular monitoring programme, or for other reasons.

## 2.3 Overview of projects and borehole investigations

Different projects involving groundwater sampling and analyses have been carried out in the Äspö HRL from 1990 to the present, i.e. construction phase 1990 to 1995, operational phase 1995 and forward. Table 2-3 presents an overview of the completed and on-going projects. Short descriptions of the projects that have produced useful hydrogeochemical data for the Äspö SDM modelling are indicated in the text below.

### 2.3.1 GWCM and F4P1 Kemimonitering

Groundwater chemical monitoring (GWCM) of the groundwater composition in isolated borehole sections has been conducted annually in selected boreholes from the ground surface since 1990 and in selected boreholes from the HRL tunnel since 1995. The monitoring programme was modified after the PLU (site investigations) and the project name changed to F4P1 Kemimonitering.

### 2.3.2 F47 kemiämnesansvar

Groundwater sampling was performed in four percussion boreholes (HAS09, HAS14, HAS18 and HAS19) in 1995 to test simple packer equipment.

### 2.3.3 REDOX

The Block Scale Redox Experiment from 1991 to 1994 involved the tunnel boreholes KFR12B, 13B and 15B and the short surface boreholes HBH01, HBH02 and HBH05 in Bockholmen Island. It consisted of a large scale natural titration experiment involving the gradual introduction of oxic groundwater to the reduced groundwater at greater depth. The samples are regarded as representative since they were collected under conditions unaffected by the experiment except for the introduction of oxygen, which is a normal process due to the presence of the tunnel. After the Redox project the sampling in the borehole sections continued as a part of the monitoring programme. In addition, Eh measurements are available from KFR12B and KFR13B.

### 2.3.4 TBM

Excavation of the last 400 m of the ‘A’ tunnel was carried out using a Tunnel Boring Machine (TBM) resulting in a tunnel diameter of 5 m. A 210 m long borehole (KA3191F) was drilled prior to the TBM drilling from the front of the blasted part of the tunnel and in the direction of the planned TBM-tunnel. Two groundwater samples from two borehole sections were collected in June 1994 before the borehole disappeared.

### 2.3.5 F64 Demoförvar

The Demonstration Repository was built to test and demonstrate the final repository techniques. Groundwater sampling was performed in borehole KZ0027A at maintained pressure and without contact with the tunnel atmosphere in order to follow possible changes when the adjacent tunnel construction proceeded. Each sample was collected in three stainless steel cylinders connected in series. Two of the cylinders were used for gas and the third for groundwater analyses (major components, ammonia, tritium, $\delta^{2}H$ and $\delta^{18}O$).

### 2.3.6 Prototype

The Prototype investigation site is located in the TBM part of the 'A' tunnel, cf. Figures 2-1 and 3-5. Experiment water samples collected in the project will not be used in the modelling. However, most of the groundwater sampling and redox measurements (Eh data) originate from several boreholes which are considered relatively unaffected by experiments and therefore suitable for modelling.

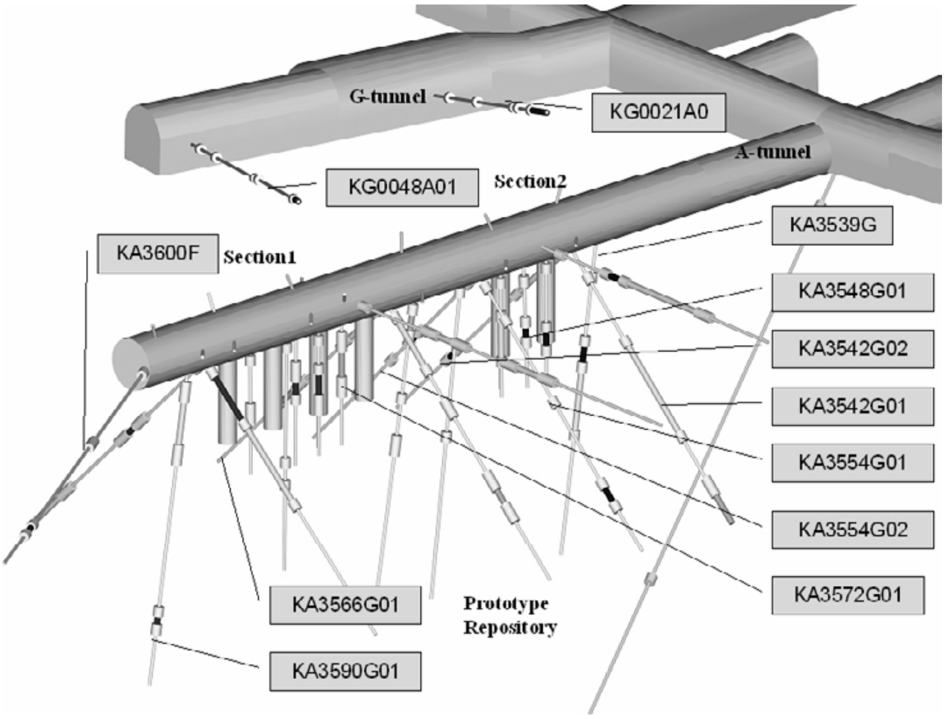

***Figure 2-1.*** *Location of groundwater boreholes outside the Prototype Repository, except for boreholes KA3566G02:2 and KA3573A:1+2 (Eriksson 2007). The boreholes KA3539G, KA3542G01, KA3542G02, KA3554G01, KA3548A01 (see Figure 3-6), KG0021A01, KG0048A01, KA3554G02 and KA3600F have measured Eh; see Section 3.2.3 and Appendix 3.*

**Table 2-3. Description of completed and ongoing projects in the Äspö HRL that entail groundwater sampling. Projects that are considered to provide representative samples for the final Äspö hydrochemical dataset have a 'Y' in the column labelled "Incl" (included). The SKB reports where more information about the different project can be found are indicated whenever possible.**

| Project abbreviation | Time period | Full project name and/or explanation | Incl Y/N | Description of groundwater sampling within the project |
|---|---|---|---|---|
| 0–750 m | 1991 | Construction of tunnel A, 0–750 m. | Y | Initial sampling mainly in short (~ 25 m) probing boreholes (SA)), see Section 6.4. |
| 750–3,191 m | 1992–1994 | Construction of tunnel A, 750–3,191 m. | Y | Initial sampling mainly in short (~ 25 m) probing boreholes (SA)), see Section 6.4. |
| GWCM | 1990–2009 | Ground Water Chemical Monitoring. | Y partly | General hydrochemical monitoring in selected surface boreholes (1990–2009) and selected tunnel boreholes (1995–2009). |
| Concrete & Clay | | | N | |
| Crock | 2011–2013 | Crystalline rock retention processes. | N | Characterisation of water to be used in laboratory experiments with drill cores and groundwaters from Äspö. |
| F47 Kemi ämnesansvar | 1995 | Hydrochemistry discipline responsibility. | Y | Groundwater sampling in four percussion boreholes in 1995 to test simple packer equipment. |
| F4P1 Kemimonitering | 2010–present | Hydrochemical monitoring. | Y | Modified monitoring programme after PLU. |
| F56 TRUE Block Scale | 1999–2002 | Tracer Retention Understanding Experiment. | Y | Aim: to improve the understanding of the transport pathways at block scale. |
| F57 REX | 1996–2001 | Redox experiment in detailed scale (Puigdomenech et al. 2001). | Y | Oxygenated water (addition in pulses) was circulated in an isolated fracture and the oxygen consumption was measured in the outgoing water. Data from KA2861A included. |
| F58 RNR | 1997– | Radionuclide Retention experiment (Jansson and Eriksen 2001). | Y | Investigation of how the rock retards and "filters" the radionuclides. |
| F60 2-phase flow | 1994– | Two Phase Flow (Jarsjö et al. 2001). | N | Study of effect of released gas on the capacity of the rock to conduct water. |
| F61 Backfill&Plug | 1998– 2003 | The Backfill and Plug Test (SKB 2003). | N | Tests of backfill materials, emplacement methods and a full scale plug. |
| F62 LOT | 1999– | Long term test of buffer material (Karnland et al. 2000). | N | Parcels with four m long copper tubes and surrounded with bentonite clay were lowered in boreholes in order to study the behaviour of the buffer at raised temperatures, thus simulating the decay heat from spent nuclear fuel. |
| F63 PROTOTYPE | 1991–ongoing | The Prototype Repository, see Section 2.3.6. | Y partly | The drilled deposition tunnel with six full-scale canisters is located in the TBM-tunnel at the –450 m level. |
| F64 Demoförvar | Nov.1996– March 1997. | Construction of the Demonstration Repository tunnel. | Y | Sampling and analyses of groundwater and gas in borehole KZ0027A. |
| F77P3 Mini Can | 1995–ongoing | Miniature canister project. *In situ* corrosion testing. | N | Samples from boreholes KA3386A02, KA3386A03 KA3386A04 KA3386A05 KA3386A06. |
| F79 LTDE | 1999–2010 | Long Term Diffusion Experiment. | Y | Samples taken during the *in situ* sorption and diffusion experiment, carried out in KA3065A03. |
| F80P1 Matrix | 1999–2010 | Matrix pore water study. | Y special | Groundwater and pore water data from the boreholes KF0051A01 and KF0066A01. |
| F82 Microbe | | Microbe project to study microorganisms and their interaction with the surroundings. | N | Special sampling setup and performance. Circulation of section water and sampling in the water line. |
| F82P1 MICOMIG | | Microbe project to evaluate the influence from microbial complexing agents and biofilms. | N | Special sampling setup and performance. Circulation of section water and sampling in the water line. |
| F82P2 MICORED | | Microorganisms and stabilisation of the redox potential. | N | Special sampling setup and performance. Circulation of section water and sampling in the water line. |

| Project abbreviation | Time period | Full project name and/or explanation | Incl Y/N | Description of groundwater sampling within the project |
|---|---|---|---|---|
| MICROBIE | | Microbial ligands in groundwater at various depth. | N | Groundwater sampling in 6 boreholes with different chemistry. General chemistry and analyses of organic species supposedly produced by microbes. |
| F83 TRUE-1 | 1994–2000 | Tracer retention understanding experiments. | N | Suspected confusion between TRUE and F83 TRUE-1. |
| F91 COLLOID | 2000–2003 | The Colloid Project. | Y partly | Stability and mobility of colloids. Bentonite clay as a source for colloid generation. Enhancement of radionuclide transport and measurement of colloid concentrations in the groundwater at Äspö. |
| F125 Alternative Buffer Material | | Study of “Alternative buffer materials” the stability of bentonites and the influence of accessory minerals in the materials. | N | |
| Hydrochemical stability | 1999–2001 | General hydrochemical investigation and evaluation programme focusing on hydrochemical stability. | – | Tube sampling (hydrochemical logging) in KLX02 1997-09-25. The water from each second tube unit was analysed. |
| KBP1001 Brytning av prototypförvaret | 2010–ongoing | Analyses of groundwater and clays. | Y | Groundwater data from boreholes in the prototype tunnel. |
| KBP4001 Undersökning av sulfidproduktion i Äspötunneln | 2011–ongoing | Sulphide production in groundwater in two boreholes in the Äspö HRL. | N | Special sampling performance to investigate sulphide production in two borehole sections in KA3110A and one in KA3385A. |
| KBS3-H | 2001–ongoing | KBS3 programme, horizontal deposition. | | |
| KLX02 | 1993–2008 | Different investigations in borehole KLX02. | – | Tube sampling in 1993-08-03 down to 1,681 m repeated in 1997-09-25.CCC in section 1,420 to 1,700 m; January 1994 and in several borehole sections down to 1,392 m during 1999 and repeated monitoring during PLU. |
| PLU | 2002–2007 | Site investigations in Forsmark and Oskarshamn. | Y partly | Selected samples from Laxemar and Simpevarp (i.e. outside the model area) will be used for comparison. |
| PRAS1001 Sulfidproduktion i grundvatten på Äspö och Laxemar | 2009–2010 | Sulphide production in groundwater from Äspö and Laxemar. | N | Special sampling performance to investigate sulphide production in KLX06, KAS03 and KAS09. |
| PREINV | 1987–1989 | Preinvestigations (1987–1989) prior to the construction of the Äspö HRL. | Partly | See Section 2.1. Selected samples from Laxemar and Simpevarp (i.e. outside the model area) will be used for comparison; see PLU. |
| The Large Scale Redox Project | 1991–1995 | The redox project. | Y | Extensive hydrochemical sampling and some Eh measurements (boreholes involved are KR0012, KR0013, KR0015, HBH01, HBH02 and HBH05). |
| Select | 1994–1996 | The project select aimed at finding suitable places in the tunnel, e.g. the REX, and the LTDE projects. | Y | 1.1.1.1 Data from boreholes KA2858A, KA3005A, KA3010A, KA3062A, KA3105A and KA3110A. |
| Select-2 | 1998–1999 | Check for suitable experimental sites along the tunnel. | Y | Data from KA 2858A. |
| SU32516 Fintätning | | | | |
| TBM | 1994 | Tunnel Boring Machine. | Y | Hydrochemical data exist (KA3191F) when drilling in the tunnel front before the use of the TBM. |
| TSF137 SWIW-test syntetiskt grundvatten | 2002–2004 | Single well injection withdrawal (Swiw) tests. | N | Study of diffusion in stagnant water, zones and in the rock matrix. Injection of synthetic groundwater. |
| TRUE-Block scale | 1999–2006 | Tracer retention understanding experiments (Tracer tests at different experimental scales). | N | Groundwater samples in Sicada – noted as F56 TRUE Block Scale or simply TRUE. |
| TUDP002 Utbyggnad Äspö | 2011–ongoing | Äspö extension project – ongoing. | Y | See Section 2.3.7 and Appendix 4. |
| ÄFS – svavel och multielement | 2004 | | Y | Data from HA1327B. |

### 2.3.7 The Äspö extension project

More space below the ground surface in the Äspö HRL is needed in order to meet the demands for research and development in connection with the construction of the intended repository for spent nuclear fuel in Forsmark, and the extension of the present repository for low and intermediate radioactive wastes (SFR). Furthermore, a new experiment location is needed for the further development of the horizontal application of the KBS-3H method. A relatively undisturbed area in the north-eastern part of the facility at around 450 m depth was judged suitable for the extension and two side tunnels were drilled, TASP and TASU (see Figure 2-2).

One of the objectives is to follow the progress of this project, evaluating the data and adapting the model of the extension volume as the project proceeds. The main reason is to explore the possibility of developing useful models at different scales for recurrent planning of future construction work and to propose important components to be included in such a modelling methodology.

At the data delivery occasion in February 2012, hydrochemical data were available from two pilot boreholes (KA2051A01 and KA3007A01). The samples were collected during drilling of the boreholes in the spring of 2011. A few elevated pH values indicate impact from grouting in some of the samples, see Section 5.2.2. Available and future groundwater data from additional new boreholes that are produced before the completion of this report are treated in Appendix 4.

## 2.4 Impacts on sampling and sampling conditions

Groundwater sampling in boreholes drilled from the HRL, or in the vicinity of the HRL, is by necessity impacted by changed hydraulic conditions due to the presence of the tunnel system as well as by additional anthropogenic activities carried out within or close to the tunnel system. In contrast to the site investigations at Laxemar and Forsmark, and in common with the dataset for the SFR-extension project (Nilsson et al. 2011), the data from Äspö will describe an artificially imposed dynamic flow system and most of the hydraulic impacts from the HRL are included in this description. In order to interpret the hydrogeochemical data correctly it is necessary to understand the hydraulic conditions and consider possible causes of sample contamination.

The possible impacts on groundwater sampling that may result in reduced sample representativeness or quality, are identified and described below. However, it should be remembered that impacts on the quality of the groundwater data (and also the quality of the chemical analyses) may, to some extent, be excluded or verified by other samples from the same borehole sections. Some of the samples represent a sample series, i.e. single samples collected from the same section at several occasions over a time period of more than twenty years, and generally show either a quite stable water composition or a clear trend due to changes in hydraulic conditions from the impact of the HRL. Besides long sample series, time series data also exist, i.e. regular and frequent samples collected during a period of days or weeks during continuous discharge from the borehole section being sampled. Time series were collected as normal routine practice from some of the boreholes included in special projects and also from the surface boreholes during the pre-investigation phase. Consistent results from sample series and sample time series increases confidence in the data.

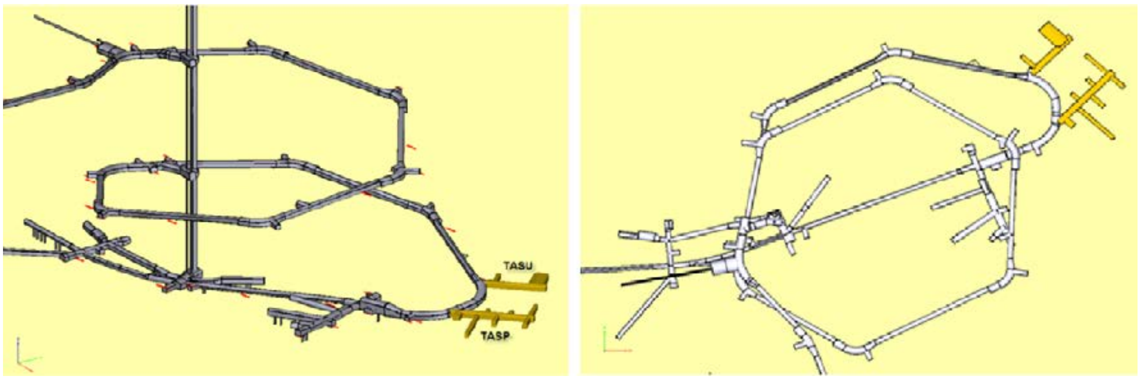

*Figure 2-2. Tunnel layout in the proposed volume for the extension of the HRL (TASP and TASU).*

### 2.4.1 Impacts from grouting

When analysing and interpreting the hydrogeochemical data from the boreholes in the HRL facility, possible impacts on the water composition from grouting should not be overlooked. Cement grouting is described in (Almén et al. 1994, Almén and Stenberg 2005). Contamination due to injection of cement increases the pH, the calcium concentration and probably also different trace metal concentrations. Furthermore, the $^{14}C$ signature may be diluted/lowered due to the addition of inorganic carbon. Elevation of pH is the most significant impact from grouting and a pH criterion is included among the quality categorisation criteria in Section 4.2. All observations of pH values ≥ 8.7 are listed in Tables 5-4 and 5-5 and possible influences from grouting are commented on.

### 2.4.2 Impacts from drilling and drilling water

Drilling of percussion boreholes, conventional boreholes and telescopic boreholes, implies, first of all, mixing of different groundwaters due to the high pressures used, and in the case of core drilling the introduction of large quantities of drilling water to cool the drill bit. Secondly, it implies impacts related to open borehole conditions following drilling when flow gradients can become established in the borehole resulting, for example, in possible short circuiting and mixing of natural groundwater flow conditions as described below. Furthermore, contamination from drilling debris and from metals due to wear and tear of the drilling equipment may occur as well.

If the pumped volume prior to groundwater sampling is insufficient, the drilling water content in the samples may remain unacceptably high. During drilling of the boreholes, uranine dye was added to the drilling water as a tracer (0.5 or 0.2 mg/L) to allow calculation of the drilling water content. Generally, adjacent percussion drilled boreholes supplied the drilling water for the core drilled surface boreholes. Two common drilling water sources for drilling the tunnel boreholes in the HRL have been KA2598A and HD0025A. KA2598A supplied the drilling water for the first two Äspö extension boreholes KA2051A01 and KA3007A01. Tap water has been used on a few occasions, for example for drilling the later Äspö extension boreholes KA3011A01 and KA3065A01. Furthermore, tap water has generally been used for grouting holes, load holes and bolt holes (200 L/min without addition of Uranine) during tunnel construction. Boreholes drilled from the HRL tunnel system, where the water flow is directed towards the tunnel, have little risk of contamination from drilling, drilling water or other borehole activities. Furthermore, many of the boreholes were drilled more than 20 years ago and possible traces of drilling water should have disappeared a long time ago.

### 2.4.3 Hydrogeological impacts

The presence of the tunnel system has an impact on the hydrogeological conditions in terms of changed flow paths and groundwater drawdown effects. These effects are observed from long term hydrochemical trends as systematic changes in the groundwater composition, i.e. dilution with modern meteoric water or marine water from the Baltic Sea or increased mixing of groundwaters of different origin. However, this has not disqualified any sample since at present they represent the groundwaters close to the HRL and therefore it is their character that needs to be explained to understand what has happened to produce these changes.

Pressure gradients (due to impact from the adjacent tunnel system) between borehole sections may cause an initial downward transport of large volumes of shallow water into new boreholes before installation of fixed packers to isolate the borehole sections. This will affect subsequent sampling and sample quality. The effect will be most pronounced in the initial samples and may gradually decrease if large volumes of water are discharged from the borehole section.

During sampling, fracture networks intersecting the boreholes may lead to short circuiting of the groundwater flow in the surrounding bedrock and also to bypassing the packer system used to isolate the borehole section being sampled. In contrast to the previously mentioned impacts this has nothing to do with the tunnel system. It means that the section sampled may have been supplied by mixed groundwaters from higher or lower levels in the bedrock, and/or mixed borehole waters above or below the packers. In both cases the sampled groundwaters when interpreted in isolation may be evaluated erroneously as being of suitable quality.

### 2.4.4 Different sampling conditions/techniques

The Äspö hydrochemical data correspond to groundwaters sampled under different conditions: different discharged volumes prior to sampling, different section lengths, different pumping techniques (surface boreholes), etc. For example, no pumping needs to be performed when sampling in tunnel boreholes since the flow direction is towards the tunnel due to pressure gradients.

Insufficient exchange of water from the borehole section prior to sampling may result in samples consisting partly of section water and partly of formation groundwater. The water initially present in the borehole section may differ considerably in composition from that of the desired formation groundwater in the bedrock. It may represent a water mixture from the entire borehole or water from different part(s) of the borehole. Plug flow calculations have been used to estimate the percentage of section water in samples from the SFR extension project cf. (Nilsson et al. 2010). Furthermore, processes might be enhanced in the isolated section, particularly if it has been packed off for some time; for example, microbial production of sulphide may be more pronounced in the borehole section compared to the surrounding water conducting fracture system in the bedrock (Tullborg et al. 2010a, b).

Samples collected from a borehole section will represent an average of the contributions from all the water yielding flow anomalies in the isolated borehole section and their different hydraulic transmissivities. Sampling from entire boreholes or long borehole sections will therefore reduce the possibility to discriminate differences in the water composition along the borehole. Furthermore, if the volume pumped out of the borehole section before sampling is insufficient to include all the anomalies in the pumped water (and this risk increases with increasing length of the sampled section, see above), the samples will also contain significant contributions of waters that have remained in the borehole for some time.

# 3 Hydrogeochemical data

## 3.1 Datasets

The Äspö hydrochemical data set contains quality assured data (see explanation in Table 1-1) from samples collected in 1) early surface boreholes during the pre-investigation phase and the later monitoring phase, 2) boreholes drilled and sampled during the construction phase of the Äspö HRL and the later monitoring phase, and 3) boreholes drilled and investigations performed for special projects in the Äspö HRL during the operational phase. The main part of the data consists of basic groundwater analyses including isotopes. However, gas, microbe and redox data are available from selected boreholes and special experiments. Quality assured data were extracted from the Sicada database (Sicada-10-077 (0:1)), complemented with late data (Sicada-12-035 (0:1)) and compiled to produce a complete Hydrochemical Data Table. This data table, in Excel format, has been reorganised in different subtables according to their future use following all the categorisation and quality analyses. This excel file is stored in the SKB documentation system SKBdoc for traceability (SKBdoc 1393008). Information on detection limits and measurement uncertainties is presented in Appendix 1.

Unless errors or questionable data were discovered during the compilation of the table, the data (values) from Sicada were not changed. But if they had to be changed, the same changes or comments on data were also incorporated in Sicada. The most frequent errors discovered during this compilation procedure concerned section limits and the corrections in Sicada are documented in Appendix 2. Some additional minor modifications to the data delivered from Sicada and stored in the Äspö final table are indicated in Chapter 7.

Apart from the information extracted from Sicada, additional columns have been added to the table either to indicate their quality (categories; the classification category are indicated numerically in a separate column) or to help with the ulterior modelling work. With respect to this last objective the additional columns contain: 1) information previously obtained during the PLU investigations (field measurements when available, microbes and gasses), 2) calculations obtained with PHREEQC (charge balance, TDS, calculated conductivity), and 3) the recalculation of parameters like silica ($SiO_2$) or sulphate (when only sulphur was available). All these columns and what they represent are thoroughly explained in one of the excel sheets in the excel file. Where microbe or gas data were available, they have been included in the corresponding sample or the sample (from the same section) closest in time, but the complete set of microbe and gas data (together with the matrix porewater samples) are compiled in three additional sheets in the same excel file. A more detailed explanation of the tables and their structure can be found in Chapter 7.

## 3.2 Available data

### 3.2.1 Groundwater samples

The hydrochemical dataset available from the Äspö investigations includes:

- 446 samples samples taken from the surface boreholes drilled within the study area (Figure 3-1). There are data from several percussion (3 from Bockholmen and 10 from Äspö[1]) and cored (1 from Bockholmen and 12 from Äspö) boreholes.
- Samples taken in the boreholes drilled from the Äspö HRL tunnel system (Figures 3-2 to 3-5; cf. Table 4-2): a) 2,295 samples from a total of 278 boreholes drilled in the tunnel. They are associated with different projects and/or experiments and will be analysed to decide which of them will be suitable for future modelling. b) 439 samples taken from weirs that may be used to evaluate inflow to the tunnel system.

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[1] There are three percussion boreholes from Laxemar inside the study area but there are not available hydrochemical data from them.

The description of the number of borehole sections, the type of samples and their categories will be included in Chapter 6 where they will finally be separated into different datasets for different purposes.

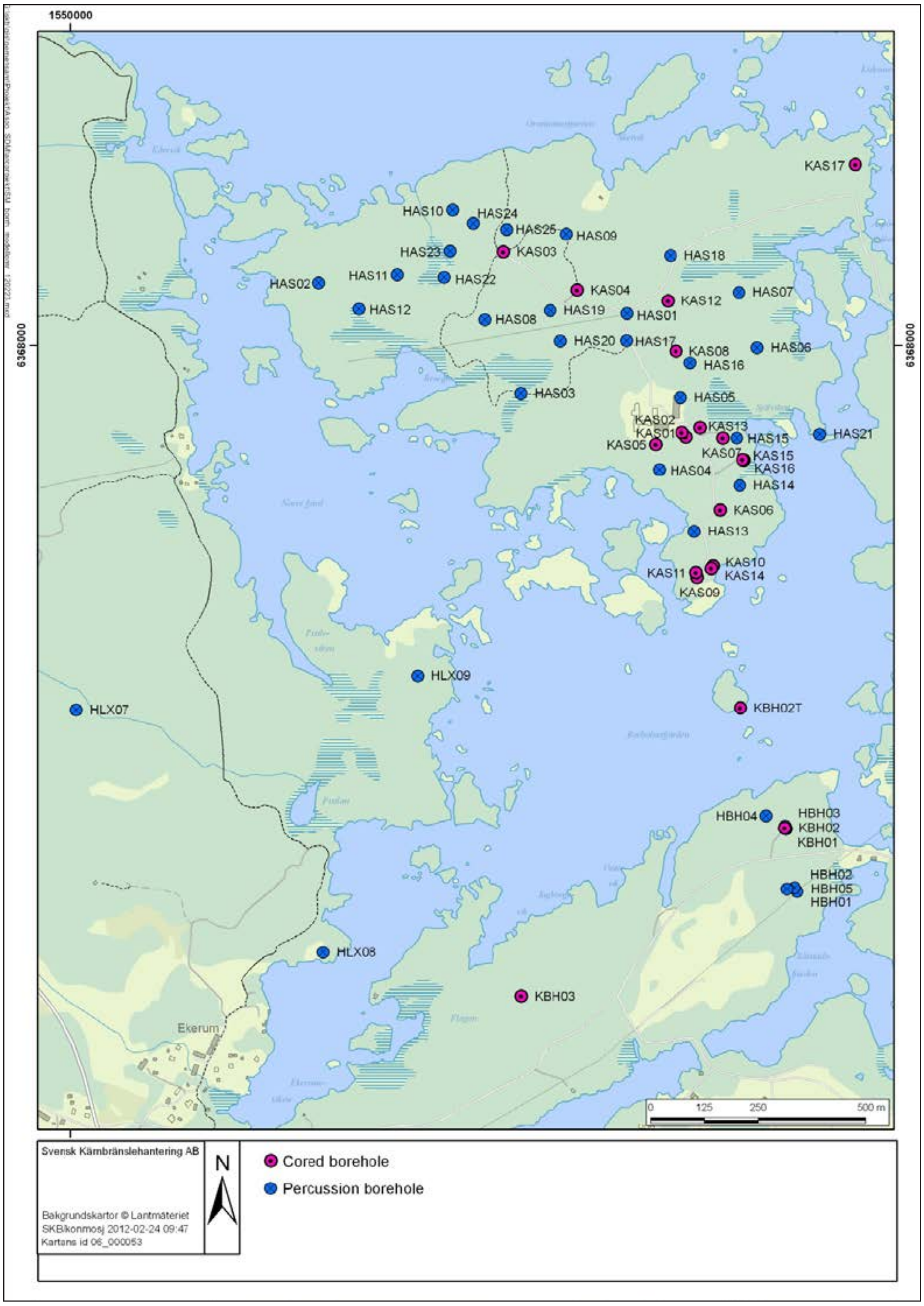

*Figure 3-1. Model area with locations of cored and percussion boreholes drilled from the surface.*

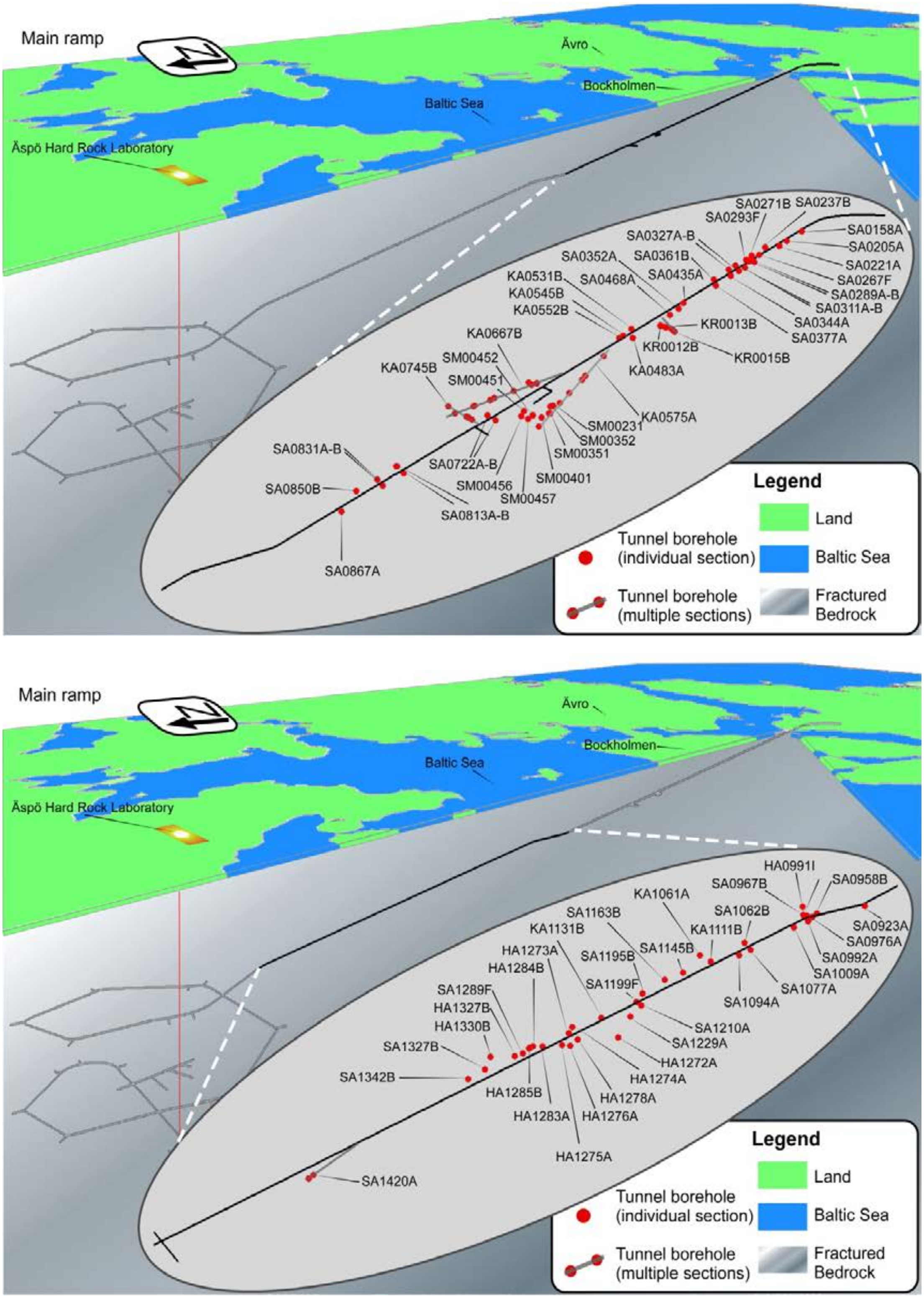

***Figure 3-2.*** *Location of the boreholes along the main ramp of the HRL tunnel.*

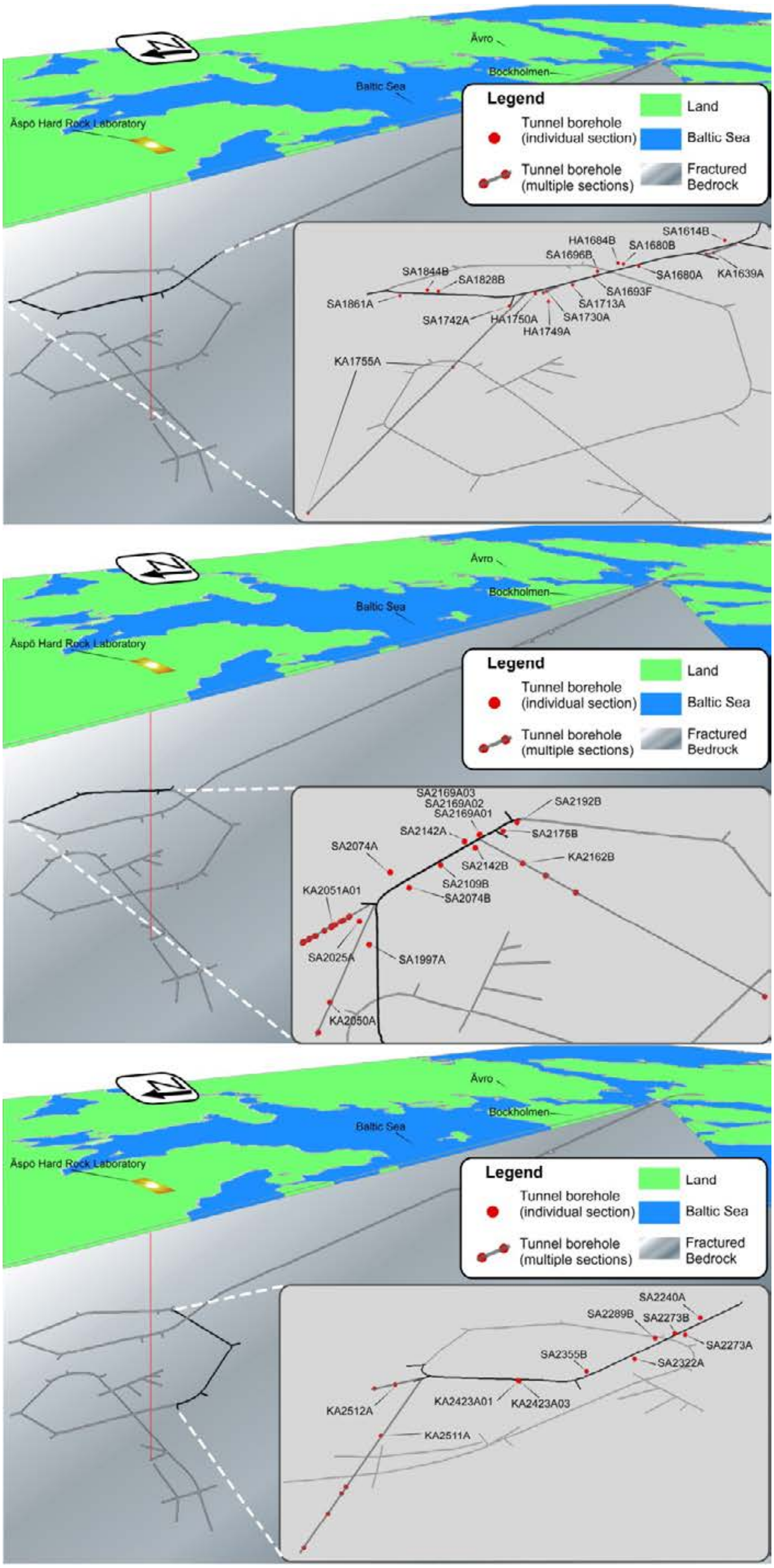

***Figure 3-3.** Location of the boreholes along the first loop of the HRL tunnel.*

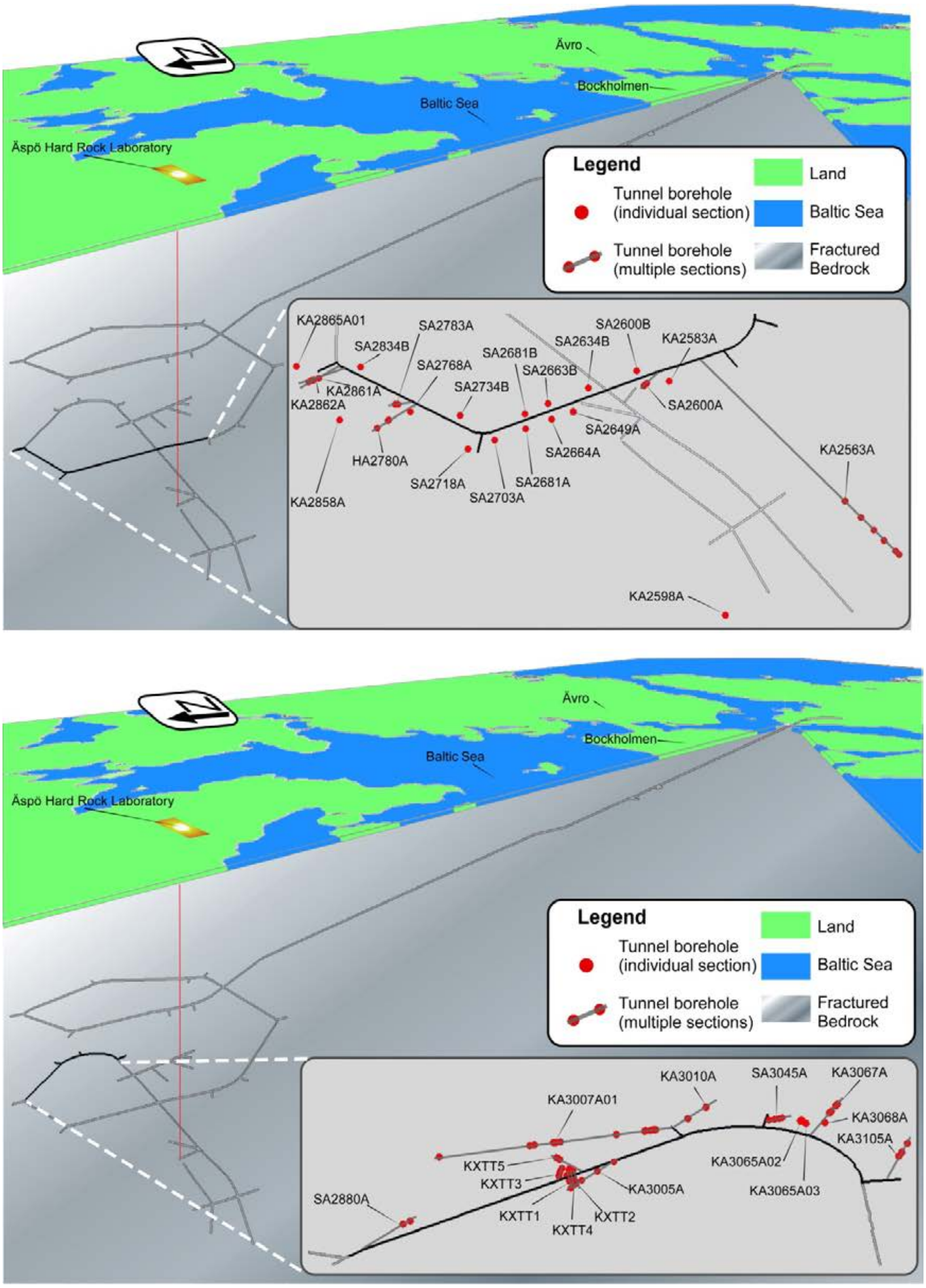

***Figure 3-4.*** *Location of the boreholes along the second loop of the HRL tunnel.*

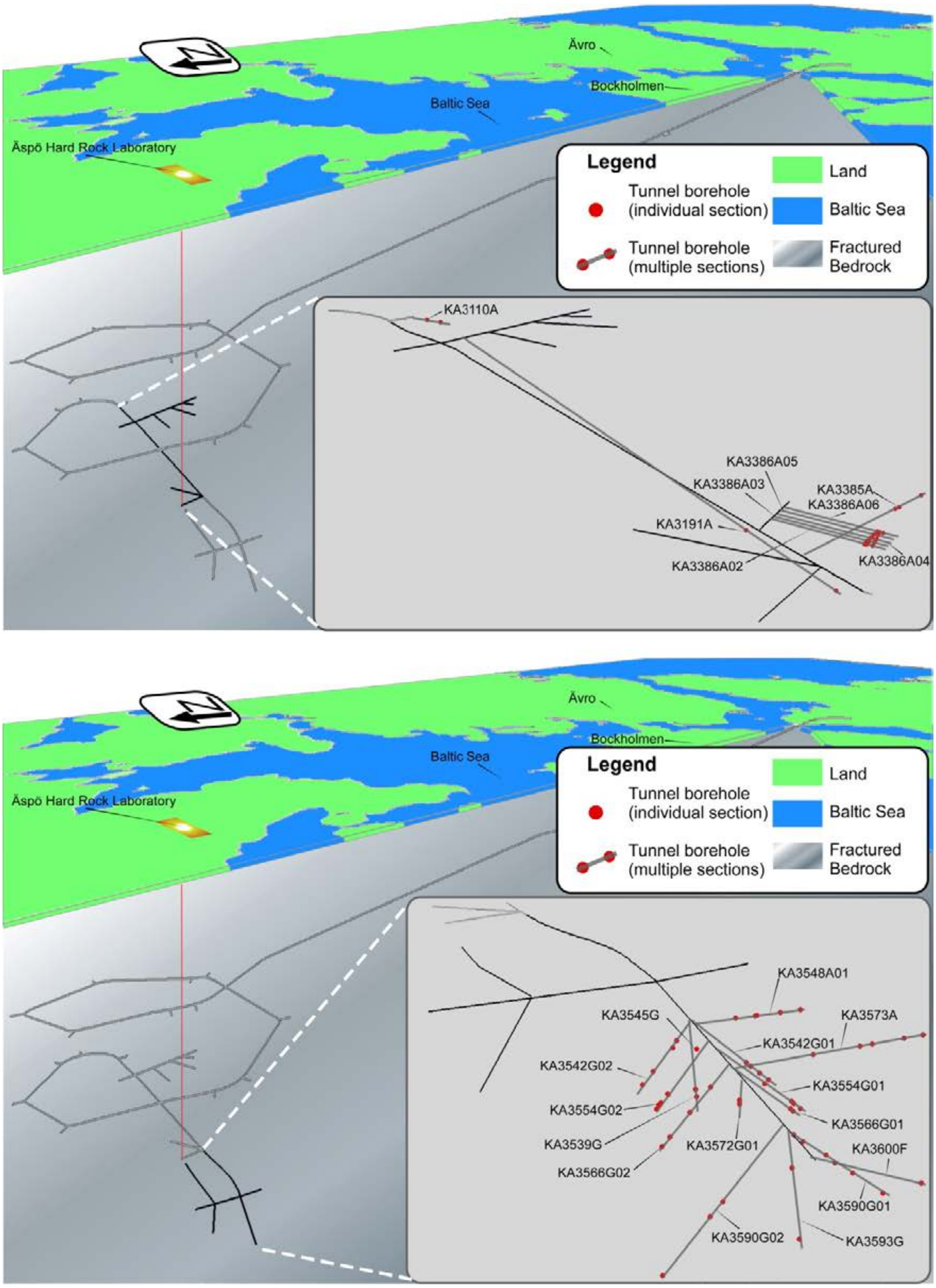

*Figure 3-5. Locations of boreholes in the last part of the HRL.*

### 3.2.2 Hydrochemical data

The analytical protocol for the groundwater chemical analysis has included mainly the same basic components and parameters from the pre-investigation phase until today. The analyses/determinations include major constituents, nutrient salts and other anions of lower concentrations, DOC and TOC, trace metals as well as stable and radioactive isotopes (see the list of parameters in Table 3-1). Several isotopes were included already during the pre-investigations ($\delta^2H$, $\delta^{18}O$, $^3H$, $^{14}C$ (pmC),

$\delta^{13}C$) and a few have been added to the protocol rather recently, especially during PLU ($^{10}B/^{11}B$, $^{87}Sr/^{86}Sr$, $\delta^{37}Cl$, $^{36}Cl$, $\delta^{34}S$). However, the full protocol has been used for a minor part of the samples and depending on the boreholes, samples and projects, the amount of data available for each sample can be quite different (for instance, many important early samples lack $\delta^{18}O$ which is an important parameter for the evaluation of groundwater origin). Considering the complete set of samples (including all the datasets compiled here), the chemical analyses that have been performed include the following:

- 786 samples contain complete chemical analyses for major and minor elements (Na, K, Ca, Mg, $HCO_3$, $SO_4$, Cl, Si, F, Br, Li, Sr, Fe(II), Mn, S(-II), N and P) and 117 of them have complete basic environmental isotopic information ($\delta^2H$, $\delta^{18}O$, $^3H$, $\delta^{13}C$ and $^{14}C$). Only 21 samples lack $^{14}C$. 386 have data for $\delta^2H$, $\delta^{18}O$ and $^3H$ and 67 only for $\delta^2H$ and $\delta^{18}O$. Still 195 samples with complete chemical analyses do not have any isotopic information or it is very incomplete.
- 1,278 samples have been analysed for complete major ions and most of the minor elements, however some of the following might be absent: Si, Br, Li, Sr, Fe(II) or Mn. Most of these samples (600) do not have any isotopic information or at the most very incomplete. However, there are 238 of these samples with data for $\delta^2H$ and $\delta^{18}O$, 404 samples which, apart from these data, also have $^3H$ analysed, and another 36 samples with the complete basic set ($\delta^2H$, $\delta^{18}O$, $^3H$, $\delta^{13}C$ and $^{14}C$).
- 87 samples lack one of the main ions (K, Mg, $HCO_3^-$, or $SO_4^{2-}$) and most of them (72) do not have any isotopic information. However, there is one sample in this group with a complete set environmental isotopic information ($\delta^2H$, $\delta^{18}O$, $^3H$, $\delta^{13}C$ and $^{14}C$), 9 samples with $\delta^2H$, $\delta^{18}O$ and $^3H$, and 3 samples with data for $\delta^2H$ and $\delta^{18}O$.
- Finally, there is also an important number of samples (968) with incomplete data for the major elements. These samples have been directly included in a separate data set (either Data Set II or Data Set IV) and have not been considered in the study. However, it is interesting to note that there is a considerable amount of isotopic information associated with these samples. For example, there are 168 samples with data for $\delta^2H$ and $\delta^{18}O$, another 100 also have data for $^3H$, and another 3 include also values for $\delta^{13}C$.

Additionally, information about the location of the samples (coordinates, metres along the borehole length, etc), the projects for which the samples were taken, and data about some laboratory measurements (pH, T, conductivity) is also available for all the samples. Density values are only available for a limited number of samples (141).

Finally, fifteen potentiometric Eh values are available from logs of on-line Eh measurements for twelve different borehole sections (Section 3.2.3). All these values have a pH measurement associated with them (although not always reliable enough to be selected). Other available redox sensitive data include: total Fe (analysed in 1,607 samples, only 4 of them b.d.l.), Fe(II) (analysed in 1,134 samples, 4 b.d.l.), S(-II) (analysed in 906 samples; 84 of them b.d.l.), Mn (analysed in 1,598 samples; only one b.d.l), N(III) (analysed in 494 samples; 200 b.d.l.), N(V) (analysed in 448 samples; 297 b.d.l.), N(III)+N(V) (analysed in 434 samples; 157 b.d.l.), N(-III) (analysed in 862 samples) and U concentrations (analysed in 257 samples; 15 b.d.l.).

Apart from the pH measurements available from the logs associated with potentiometric Eh measurements, most of the available pH data were measured in the laboratory and this situation may represent a serious uncertainty in redox pair modelling and speciation-solubility calculations. Field measurements of pH have been conducted only at recent monitoring occasions (172 samples with field pH data) and/or in connection to redox measurements. Conductivity and temperature were also measured in the laboratory, but there are several samples in which these two parameters were also measured in the field (115 temperature measurements and 101 conductivity measurements).

For a general idea of the contents and distribution with depth, and the chloride content of some of the main parameters in the final data set, some plots can be found in Chapter 7.

During the pre-investigations most of the basic analyses were conducted in the SKB mobile chemistry laboratory (Almen and Zellman 1991) located at the drill site close to the investigated borehole, and duplicate samples were sent also to one or two external laboratories as a check (initially AAS and flame emission, later on ICP-AES). ICP started to be the dominating technique since the end of the 1980's, subsequently replacing AAS, flame emission, ion chromatography, EDTA-titration and spectrophotometric methods for cations. With respect to the isotopic analyses, the most important improvements during the time period 1986 to 2011 are the lowered detection limit for tritium by sample electrolysis (enhanced) and the change of method for $^{14}C$ from LSC to accelerator measurements.

Following the inauguration of the well equipped Äspö chemistry laboratory in 1995, the analyses were no longer conducted in the mobile field laboratory. The distance from the HRL and the surface boreholes at Äspö, Laxemar and Simpevarp is short underlining the suitability of the laboratory for those analyses that need to be conducted immediately ((Fe(II), Fe-tot, $NH_4$, $HCO_3$ and lab-pH). The basic analyses and analytical methods are listed in Table 3-1.

**Table 3-1. Components/isotopes and methods.**

| Component | SKB methods, mobile laboratory and Äspö chemistry laboratory | External methods and analyses |
|---|---|---|
| pH-lab, EC-lab* | Conventional SS | – |
| Na, K | Ion chromatography** | ICP-AES (Na, K, Ca, Mg, Fe, Mn, Si, Li, Sr, S-tot, Br, I)*** |
| Ca, Mg | EDTA-titration** | |
| Mn | Spectrophotometry SS** | |
| Si, S-tot, Fe, Li, Sr, Br, I*** | – | ICP-AES*** |
| Fe(II), Fe-tot | Spectrophotometry-Ferrozine, Fe(II), Fe-tot | – |
| $HCO_3$ | Titration SS | – |
| Cl | Mohr-titration (recently with IS-electrode), Ion chromatography | – |
| Br | Ion chromatography | ICP-AES |
| F | Ion chromatography, potentiometric method | – |
| $SO_4$-S | Ion chromatography | ICP-AES (S-tot) |
| $NO_3$-N, $NO_2$-N, $NH_4$-N | Spectrophotometry SS | Spectrophotometry SS ($NO_3$-N, $NO_2$-N, $NO_3$+$NO_2$-N) |
| $PO_4$-P | | Spectrophotometry SS |
| $SiO_2$ | | ICP-AES (Si) |
| $S^{2-}$ | | – |
| I | – | ICP-AES/MS |
| TOC, DOC | – | Carbon analysator |
| Other trace metals, including REEs | – | ICP MS High resolution / ICP MS |

| Isotope | Methods 1986–2001 | Methods after 2001 |
|---|---|---|
| Tritium | LSC, DL=8 TU<br>Electrolysis+LSC, DL=0.8 TU (few values) | Electrolysis+LSC, DL=0.8 TU |
| Deuterium | MS | |
| $\delta^{18}O$ | | |
| $^{14}C$ (pmC) | Release of $HCO_3$ from 130 L water in the field. LSC. Carbon-14 age and age corrected for $^{13}C$. A few AMS values | AMS |
| $\delta^{13}C$ | MS | |
| Uranium isotopes | AS | AS, ICP MS |
| Thorium isotopes | | AS, ICP MS |
| $^{222}Rn$ | LSC | |
| $^{226}Ra$ | | |
| $^{10}B/^{11}B$ | – | ICP MS |
| $^{87}Sr/^{86}Sr$ | – | TIMS |
| $\delta^{37}Cl$, | – | MS |
| $\delta^{34}S$ in sulphate**** | – | MS |

* Field measurements of pH are available only in connection with long term Eh measurements; see Section 3.2.5.
** These methods were not used after about year 1990. *** Before 1989 AAS was used for some of the cations.
**** Some determinations of $\delta^{34}S$ in sulphide exists.

**Abbreviations:**

| | | | |
|---|---|---|---|
| ICP AES | Inductively Coupled Plasma. Atomic Emission Spectrometry | LSC | Liquid Scintillation Counting |
| AAS | Atomic Absorption Spectrometry | MS | Mass Spectrometry |
| SS | Swedish Standard method | AS | Alfa Spectroscopy |
| INAA | Instrumental Neutron Activation Analyses | AMS | Accelerator Mass Spectrometry |
| ICP MS | Inductively Coupled Plasma Mass Spectrometry | TIMS | Accelerator Mass Spectrometry |
| REES | Rare Earth metalls | | |

### 3.2.3 Measured Eh and pH data

On line measurements of Eh and pH are available from seven borehole sections in surface boreholes and from 34 tunnel borehole sections in the HRL. The logs from the surface boreholes have been thoroughly evaluated in Auqué et al. (2008) and the selected representative Eh and pH values for each specific borehole section are presented in Table 3-2.

The logs from the HRL boreholes, on the other hand, have not been subjected to the same careful analysis and will be evaluated in detail below. On-line measurements of Eh and pH in the tunnel boreholes have been performed mainly within three different projects using three different equipment types:

- Redox project, between 1991 and 1993 (Banwart et al. 1994).
- REX project, a continuation of the Redox project in 1998 (Puigdomenech et al. 2000).
- Prototype project between 2006 and 2010 (Pedersen et al. 2004).

In the Redox project Eh and pH measurements (and dissolved oxygen, EC and groundwater temperature) were conducted in boreholes KR0012B and KFR0013B, using the Surface Chemmac system which was situated in the so-called hose unit (Almén and Zellman 1991) located in the Redox tunnel close to the borehole orifices. The outlets from the boreholes were connected via Tecalan tubing to the surface Chemmac measurement cell which maintained a pressure of 1.5 to 2 Bars. The Eh and pH measurement sequences from these relatively shallow locations are presented in Figures A3-1 and A3-2 in Appendix 3. The selected Eh and pH values are given in Table 3-3.

The Prototype measurement cell was designed especially for the Prototype project. The inner part of this cell, as well as the dummy included to reduce the section volume, is made of PEEK (Polyether ether ketone). Furthermore, PEEK tubing was used to connect to the borehole water outlet in order to minimise possible oxygen diffusion. The idea was to maintain the pressure from the sampled borehole section as close as possible in the measurement cell. The major part of the Eh data from the HRL boreholes is available from this project. The ten boreholes with Eh measurements are located between 430 and 470 m depth in the vicinity of the Prototype experiment site; Eh and pH measurement sequences are presented in Figures A3-3 to A3-12 in Appendix 3. The selected Eh and pH values from each presented measurement sequence are given in Table 3-3.

**Table 3-2. Selected representative Eh and pH values measured during the pre-investigation phase in surface boreholes in the Äspö model area, modified after (Auqué et al. 2008). (Boreholes outside the model area are omitted).**

| Borehole | Date | Sample | Section (m) | Elevation (m.a.s.l.) | Eh (mV) | pH |
|---|---|---|---|---|---|---|
| KAS02 | 11/01/1989 | 1548 | 212–214 | –199.81 | –257 | 7.5 |
| | 11/04/1988 | 1418 | 314–319 | –307.69 | –380 | 8.45 |
| | 04/05/1988 | 1432 | 530–535 | –522.95 | –310 | 8.35 |
| KAS03 | 21/02/1989 | 1569 | 129–134 | –121.78 | –260 | 8.0 |
| | 15/03/1989 | 1582 | 860–1,002 | –914.04 | –270 | 7.3 |
| KAS04 | 17/04/1989 | 1596 | 226–235 | –185.15 | –300 | 7.8 |
| | 27/04/1989 | 1603 | 334–343 | –275.61 | –280 | 7.9 |

Generally, the redox measurements were successful and resulted in quite reasonable and reliable Eh values. However, several measurements were interrupted due to technical problems which caused breaks in the trends. All the evaluated Eh values indicate mildly reduced conditions between –110 and –220 mV. The highest values –110 to –150 mV were obtained in the shallowest boreholes KR0012B and KR0013B, but also KA3600F at 446 m depth showed a similar redox potential.

**Table 3-3. Selected Eh and pH values from tunnel boreholes (Redox and Prototype projects) with comments on the selection. See Appendix 4 for plots**

| Borehole | Sample | Date | Section (m) | Elevation (m.a.s.l.) | Eh (mV) | pH |
|---|---|---|---|---|---|---|
| KR0012B | | 1991 | 5.04–10.57 | –69.17 | –110±20 | 7.7±0.12 |
| | (*) | Acceptable Eh and pH measurements. The Eh electrodes diverge; the platinum and gold electrodes show reasonable agreement within the error. No selected values in Sicada, but they have been included in all the samples from the same section and date. | | | | |
| KR0013B | | 1991 | 7.00–16.94 | –69.22 | –130±20 | 7.5±0.2 |
| | | 1993 | 7.00–16.94 | –69.22 | –150±30 | 7.35±0.15 |
| | (**) | Acceptable Eh and pH measurements. The pH varies quite much during 1993. No selected values in Sicada, but they have been included in all the samples from the same section and dates (1991 and 1993, respectively). | | | | |
| KA2512A | | 2006 | 0–37.27 | –336.37 | –221±16 | 7.5±0.2 |
| | | 2006 | 0–37.27 | –336.37 | –200±30* | 7.6±0.8* |
| | | Acceptable Eh and first pH measurement. The second pH sequence is difficult to interpret. The second selected values from the later measurements are changed compared with the selected values in Sicada (–175 mV and 7.0, respectively) to better agree with the initial measurements. | | | | |
| KA3539G | | 2006 | 15.85–17.60 | –465.73 | –170±25 | 6.8±1.2 |
| | | Acceptable Eh measurement. The pH curve varies between 6.7 and 8.0. Varying calibration constants cause large error in pH. | | | | |
| KA3542G02 | | 2007 | 25.6–27.2 | –467.17 | –167±26 | 7.4±0.4 |
| | | Acceptable Eh and pH measurements. The pH curves diverge slightly. An average value is selected but there is not a sample from that date to which these values could be associated with. The relatively large error is due to uncertain calibration constant. | | | | |
| KA3542G01 | 14026 | 2007 | 18.6–20.3 | –462.78 | –196±42 | 7.5±0.3 |
| | 20513 | 2010 | 18.6–20.3 | –462.78 | –153±15 | 7.2±0.3 |
| | | Repeated measurements. Acceptable Eh and last pH measurements. The selected average values from Sicada are considered representative. | | | | |
| KA3554G01 | 14022 | 2007 | 22.6–24.2 | –465.39 | –183±79 | 7.3±0.5 |
| | | Acceptable Eh measurement. The selected average value from Sicada is considered representative. pH starts at 7.5 and 7.3 and ends at close to 7.0, i.e. large uncertainty (value not selected for modelling). | | | | |
| KA3548A01 | 14024 | 2007 | 8.8–10.80 | –447.11 | –170±20* | 7.0±0.4 |
| | | Difficult to interpret Eh and pH. The Eh value is reasonably well defined but the two diverging pH measurements show steady slopes. | | | | |
| KG0021A01 | | 2008 | 35.0–36.0 | –434.38 | –187±42 | 7.24±0.5 |
| | | Three stable and agreeing Eh electrodes, average value selected but there is not a sample from that date to which these values could be associated with. The pH measurement sequence is irregular and unstable with values between 7.2 and 7.4. | | | | |
| KG0048A01 | | 2008 | 32.8–33.8 | –436.43 | –203±31 | 7.3±0.8 |
| | | Three rather stable but somewhat disagreeing Eh electrodes, average value selected but there is not a sample from that date to which these values could be associated with. The pH sequence is stable at 7.3 pH units but the uncertainty is large due to uncertain calibration constant. | | | | |
| KA3554G02 | | 2008 | 10.5–12.2 | –456.84 | – 170±13 | 7.2±0.4 |
| | | Parts of the Eh measurement sequences show three stable and agreeing Eh electrodes. However the pH measurement shows a sloping trend starting at pH> 8.0 and ending with stable readings close to pH=7.2. | | | | |
| KA3600F | 20521 | 2010 | 40.5–42.0 | –446.81 | –150±11* | 7.34±0.3*** |
| | | A short period with stable and agreeing Eh electrodes at –150 mV. pH was also stable during the same period at 7.34. | | | | |

* The selected value has been introduced in the final table for all the samples corresponding to the same section and the same year (1991).

** The selected value has been introduced in the final table for all the samples corresponding to the same section and the same year (1993).

*** Different selection than the one indicated in Sicada.

The corresponding pH measurements, on the other hand, were less successful and the evaluation of representative values is difficult and uncertain. This may be due to the high resistivity of the glass membrane in glass electrodes which makes them more sensitive to electrical disturbances compared with the metal electrodes used for Eh measurements. The electrical environment in the tunnel system is quite complicated and may be the reason for undesired impacts on the pH measurements. The selected pH values for the different borehole sections cover a rather narrow range varying between 7.0 and 7.7 pH units. Plotted measurement sequences are presented in Appendix 3 except for the REX results whose measurements were affected by oxygen pulses and they are of less use for modelling purposes.

### 3.2.4 Colloid-, microbe- and gas data

#### *Colloid data*

The colloid data from the Äspö area (including Laxemar and Simpevarp) have been obtained by seven different methods; cf. Table 3-4. Four of these methods were used during PLU and the dataset only includes samples from boreholes in Laxemar (less relevant for Äspö). One method "Colloid measurements" was used in a special colloid project (F91 Colloid) in the HRL tunnel to investigate colloid generation from bentonite but the results are not representative of natural conditions in the groundwater (Laaksoharju and Wold 2005). Furthermore, data obtained by the early method "Sampling of particulate matter" are questionable since they imply filtering through a series of connected filters in the presence of atmospheric oxygen.

The most useful colloid data for the Äspö dataset are the thirteen measurements obtained by LIBD (Laser Induced Breakdown Detection). They were also obtained within the F91 Colloid project but the intention was to measure the natural background content. These measurements were conducted on two occasions (October 2001 and October 2004) by using mobile equipment connected directly to the borehole outlet tubing and therefore should represent conditions as undisturbed as possible if the unavoidable discharge from the borehole section is disregarded. Figure 3-6 shows the colloid content (µg/L) *versus* chloride concentration and may be used to give a general rough estimate of the colloid content in the Äspö HRL groundwaters.

**Table 3-4. Summary of colloid studies performed in the Äspö area (including Laxemar and Simpevarp).**

| Activity type (sampling method) | Äspö SDM data | No records | Explanation | Time period | Sampling locations |
|---|---|---|---|---|---|
| Colloid filtration | No | – | PLU method | – | Laxemar |
| Colloid measurements | Yes | 100 | Studies performed in the Colloid project with bentonite as a source for colloid generation | 2007-11-27 to 2009-02-25 | HRL and KAS09 |
| Colloid measurements using LIBD | Yes | 13 | Mobile equipment for Laser Induced Breakdown Detection | 2001-10-01 and<br>2004-10-31 to 11-02 | HRL |
| Fractionation of colloidal metals | No | – | PLU method | | Laxemar |
| Sampling of particulate matter | Yes | 18 | Filtering through a series of connected filters | 1988-04-09 to 2001-10-23 | HRL, AS |
| SEM colloid measurements | No | – | PLU method | – | Laxemar |
| Fractionation of humic and fulvic acids | No | – | PLU method | – | Laxemar |

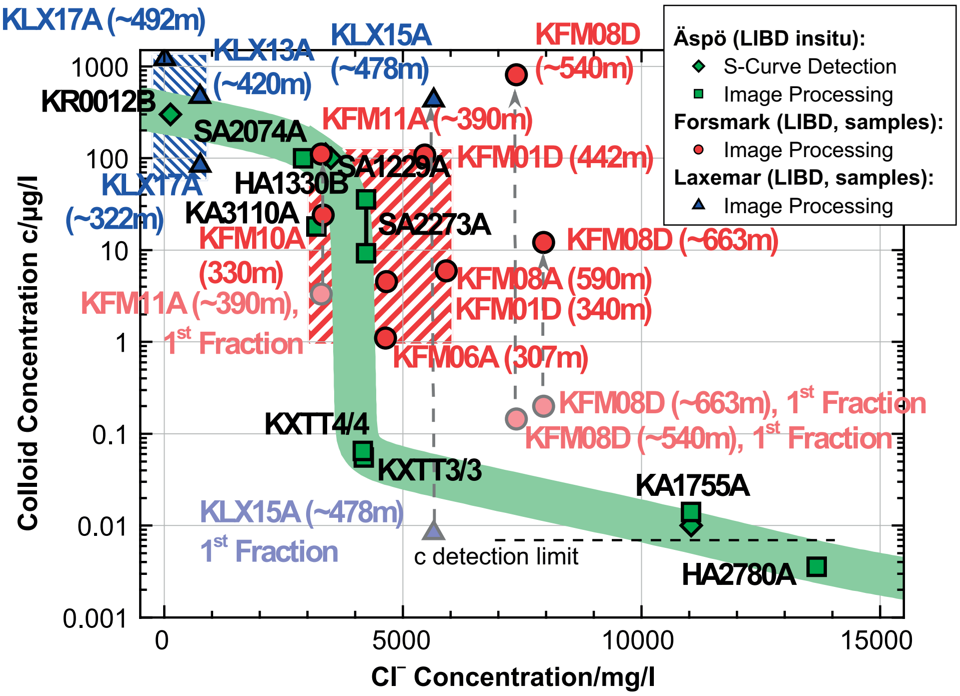

***Figure 3-6.*** *LIBD analysed colloid concentration as a function of the Cl-concentration (Laaksoharju and Wold 2005). Data points connected by bars indicate varying concentrations due to pressure fluctuations. Data from site investigations in Forsmark and Laxemar are included for comparison. These are not measured in situ and show much more variation.*

### *Microbe data*

Microbiological data are available for 116 samples (although not all of them contain data for all the parameters). However, only 45 of them have an associated sample with more or less complete chemical analyses. These data include determinations of total number of cells, concentration of ATP, number of cultivable metabolic groups, heterotrophic aerobic bacteria, and most probable number of cultivable metabolic groups, i.e. iron, manganese, sulphate and nitrate reducing bacteria, as well as acetogens and methanogens.

There are 103 samples taken from 37 boreholes drilled in the tunnel: 40 of them correspond to 13 boreholes drilled for the Prototype project (PXP boreholes) and only 7 of these samples have an associated chemical composition. The other 63 samples were taken in 24 different boreholes in the tunnel associated with the projects Micomig, Mini-Can, Prototype, Microb and SGU Tracertest. Only 33 of them have associated chemical analyses. Finally, there are 13 samples taken from the two surface boreholes in Bockholmen but only the information on the total number of cells is available and there are no chemical analyses associated.

Figure 3-7 and 3-8 show the distribution with depth of several microbial parameters and may be used to give a general rough estimate of their content in the Äspö HRL groundwaters. Data from samples taken during the site investigations at Laxemar and Simpevarp are also shown for comparison.

The whole set of microbial data has been compiled in a separate sheet in the final excel file named “Allmicrobes”. The data corresponding to water samples with a complete chemical characterisation have been included in the corresponding data set tables in the general excel book.

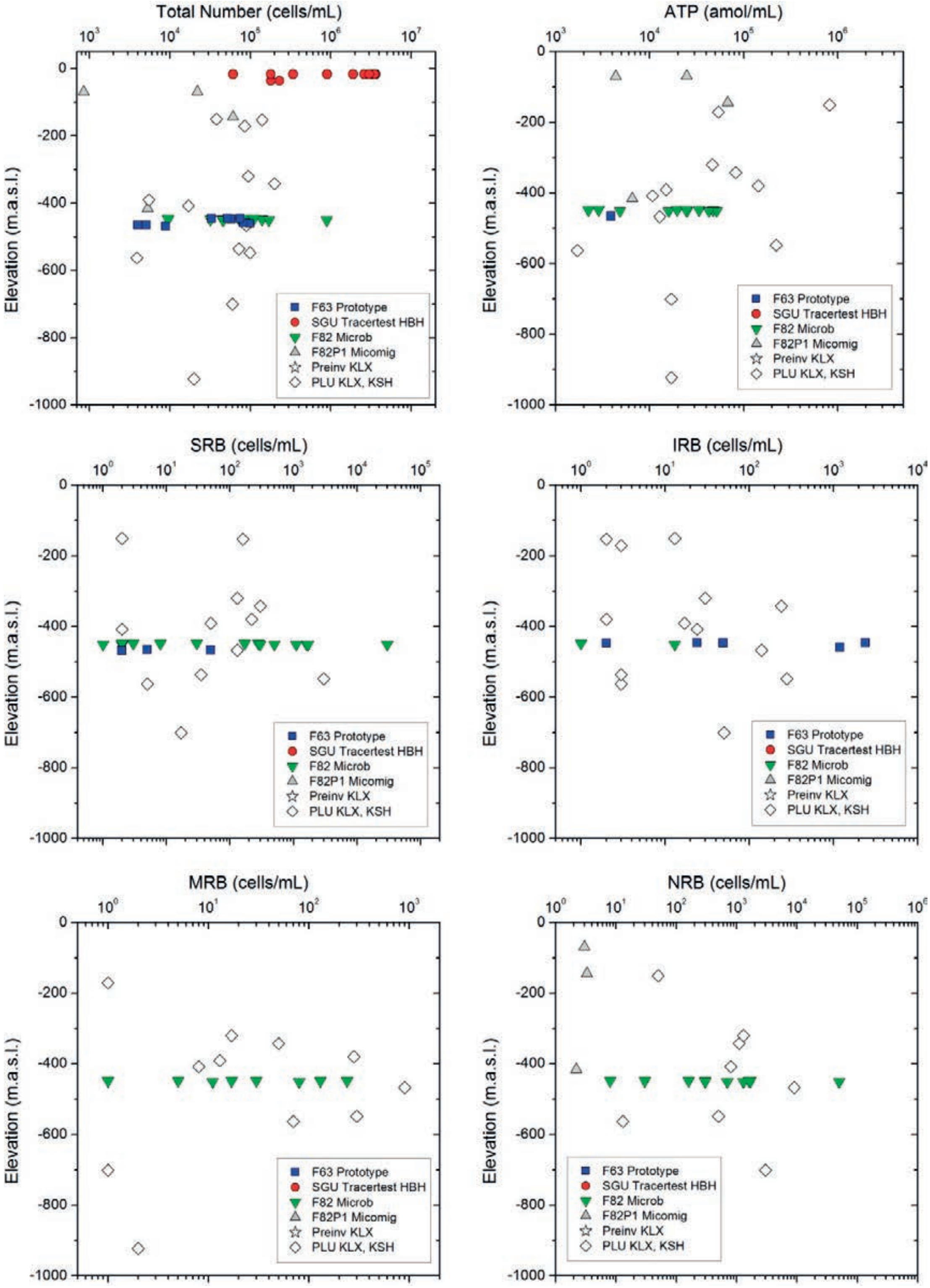

*Figure 3-7. Distribution with depth of several microbial parameters in the Äspö groundwaters. The samples are colour coded as a function of the project within which they were taken and analysed. Data corresponding to Laxemar (PLU KLX) and Simpevarp (PLU KSH) groundwaters are also shown for comparison.*

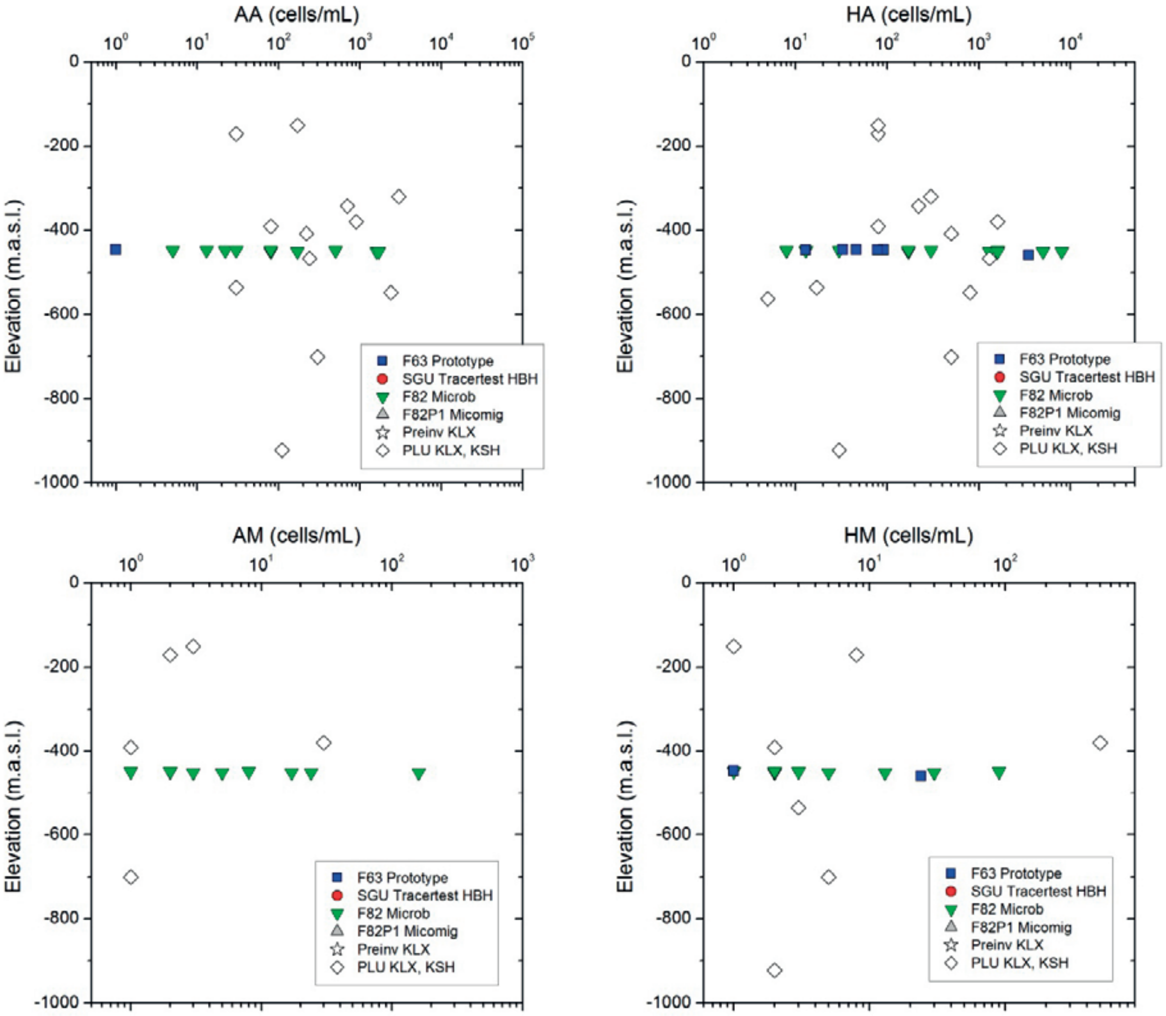

*Figure 3-8. Distribution with depth of several microbial parameters in the Äspö groundwaters. The samples are colour coded as a function of the project within which they were taken and analysed. Data corresponding to Laxemar (PLU KLX) and Simpevarp (PLU KSH) groundwaters are also shown for comparison.*

### Gas data

Gas data, including gas compositions ($N_2$, $H_2$, $CO_2$, $O_2$, Ar, $CH_4$, He, CO, $C_2H_2$, $C_2H_4$, $C_2H_6$ and $C_3H_8$) and the total gas volume, are available for 204 samples taken from several boreholes:

1. There are 181 samples taken from 10 boreholes drilled in the tunnel:
   - 17 samples were taken in 6 boreholes along the tunnel associated with the projects Micomig, Prototype, Micored, Select and "Kemiämnesansvar". Only 4 of them have associated chemical analyses.
   - The rest of the samples (164) were taken in only 4 boreholes. Three of them were mainly associated with the Microb project: KJ0050F01 (18 gas analyses but only 3 with associated chemical analyses), KJ0052F01 (49 gas analyses but only 7 with associated chemical analyses) and KJ0052F03 (73 gas analyses but only 2 with associated chemical analyses). The fourth borehole (KZ0027A) has 24 analyses corresponding to two duplicates of 12 samples with chemical analyses; the two subsamples were sent to different laboratories for check. All the data are associated with the F64 Demoförvar project.
2. There are seven samples taken from three surface boreholes at Äspö (during the Pre-investigation phase) and all of them have groundwater samples associated with complete chemical analyses.

A general overview of the data is shown in Figure 3-9 with the distribution of the main gas types with depth. Data from Laxemar and Simpevarp are also shown for comparison.

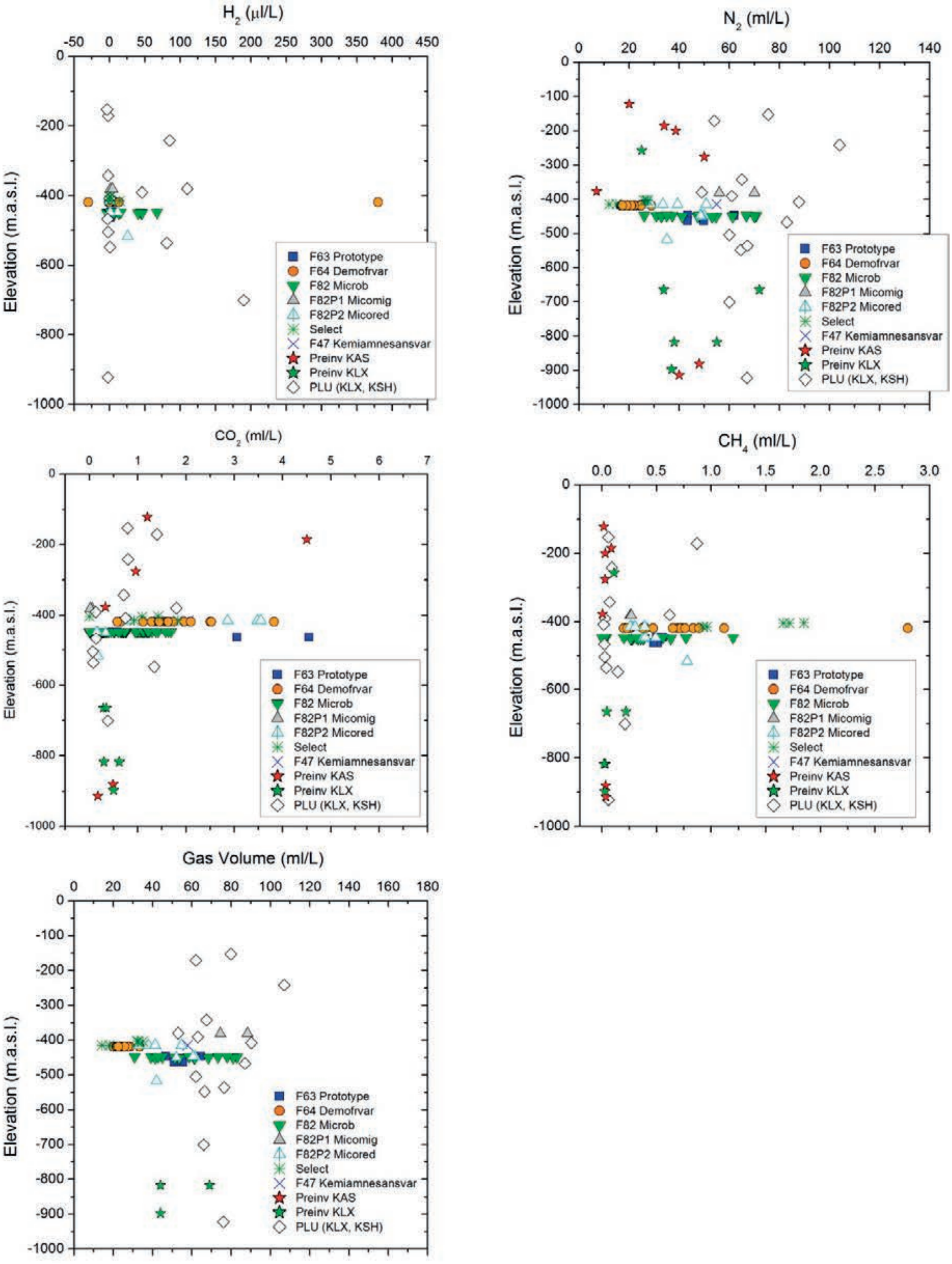

***Figure 3-9.** Gas content distribution with depth in the Äspö groundwaters. The samples are colour coded as a function of the project within which they were taken and analysed. Data corresponding to Laxemar (PLU KLX) and Simpevarp (PLU KSH) groundwaters are also shown for comparison.*

It is important to indicate at this juncture about the data delivered by Sicada under the column for oxygen gas. The presence of $O_2$ gas in the samples is an artefact due to the intrusion of air into the sample during sample handling or the gas extraction procedure. The reporting of analytical results for dissolved oxygen to the Sicada database has varied from time to time and three different strategies have been used:

- The $O_2$ concentration is recorded among the other gas analyses in Sicada.
- The $O_2$ concentration is removed as well as the corresponding $N_2$, $CO_2$ and argon concentrations calculated from the $O_2$ concentration.
- Both records are given for the sample, i.e. including the intruded air, and excluding the air corresponding to the $O_2$ concentration. As indicated in the final remarks in Chapter 8, it is recommended to give these two records.

The whole set of gas data has been compiled in a separate sheet in the final Excel file named "Allgases". The data corresponding to water samples with a complete chemical characterisation have been included in the corresponding dataset tables.

### 3.2.5 Matrix porewater data

#### *Background*

'Matrix pore-water' refers to the water present in the connected pore space of the rock matrix that is accessible for interaction with groundwaters circulating in nearby fractures. Attempts to study these pore-waters were carried out on two occasions at the Äspö HRL (Smellie et al. 2003, Waber and Smellie 2008).

Prior to the first occasion, little was known about the composition and evolution of rock matrix pore-waters in crystalline rocks; Canadian studies indicated porewaters of high salinity approaching brine composition (> 100 g/L) (Gascoyne et al. 1996). The main objective, therefore, was to understand the origin and age of pore-waters sampled in the connected rock matrix pore space and in micro-fractures and to determine their possible influence on the chemistry of the groundwater from the surrounding, more highly permeable bedrock. This was carried out in Borehole KF0051A01, of total length 11.70 m, drilled at an upwards inclination of ~ 30° from Tunnel 'F' at a depth of about 450 m in the Äspö HRL (cf. Figure 3-10). For this study the term 'matrix pore fluid' was used to include the following fluid types: a) the water in the pore space of a rock that is only accessible by diffusion, b) the water residing in dead-end pores, and c) the fluid enclosed in mineral fluid inclusions. The term 'matrix pore-water' was used when referring to the water in the connected pore space of the rock matrix that is accessible for interaction with groundwaters circulating in nearby microfractures.

Water sampling was carried out at five occasions during two major sampling stages: a) three occasions to sample matrix pore fluids from water present in the pore space of the unfractured bedrock matrix (i.e. Figure 3-10), and b) two further occasions from nearby bedrock matrix containing small microfractures exposed when the packer system in Figure 3-10 was moved some 90 cm towards the tunnel face. When the second investigation was conducted some two years after completion of the initial study, extraction of matrix pore-waters under laboratory conditions had been tested and found promising for the on-going PLU investigations at Forsmark and Laxemar. This new approach was considered necessary as it was both impractical and time consuming to conduct long term direct sampling and analysis of matrix pore-waters similar to that described for Borehole KF0051A01. Emphasis was therefore put on the rock matrix itself, focussing on suitable method(s) to rapidly extract and chemically characterise the accessible matrix pore-water from unfractured drillcore lengths (cf. Waber and Smellie 2008).

However, this approach gave rise also to potential difficulties and uncertainties, one of which was the possible contamination of the pore-water during drilling and extraction of the investigation boreholes. This resulted in locating another underground locality at the Äspö HRL to examine the effects of the drilling process and related potential contamination of the pore water by drilling fluid. This was carried out in borehole KA3386A06 (cf. Figure 3-11) which represented the last of six horizontal boreholes drilled to install miniature copper capsules to study the effects of long-term copper corrosion (i.e. the 'Copper Canister Project').

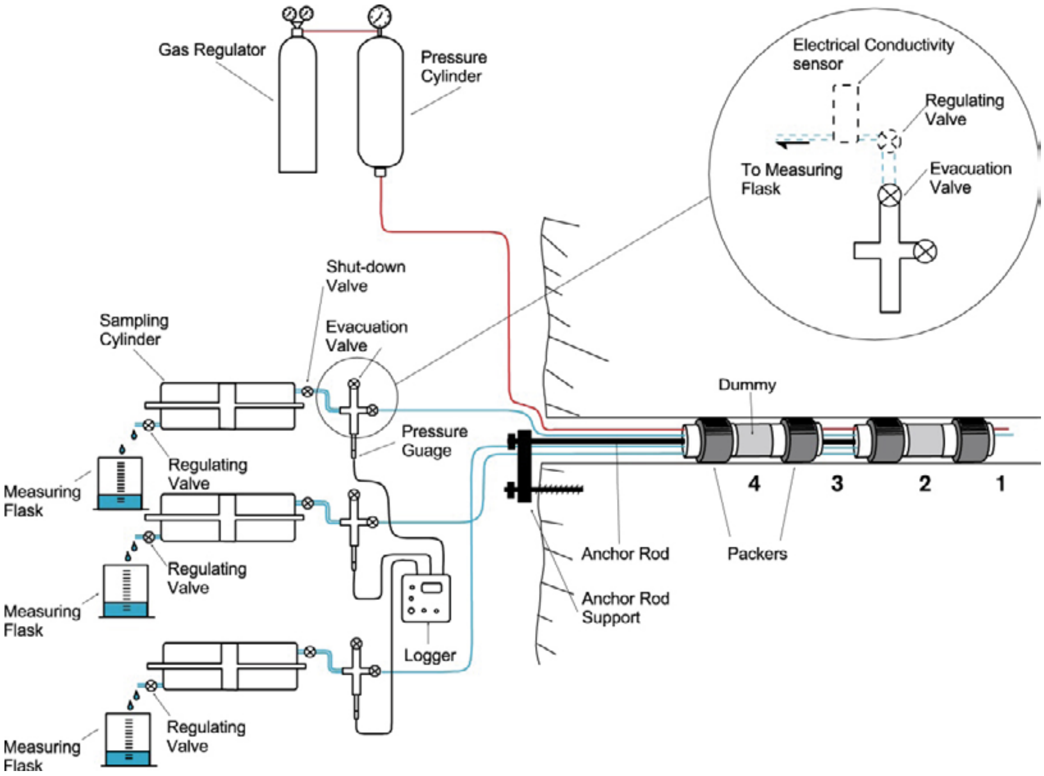

***Figure 3-10: Matrix Fluid Chemistry Experiment (MFE) set-up.*** *Borehole KF00051A011 sections 2 (8.85–9.55 m) and 4 (4.66–5.26 m) were specifically selected to collect matrix pore-water, however section 3 (6.26–7.85 m) was also successfully sampled; Section S1, with the highest residual volume, could only be sampled for gas. The contact between Äspö diorite and Ävrö granite occurs at 8.5 m from the tunnel.*

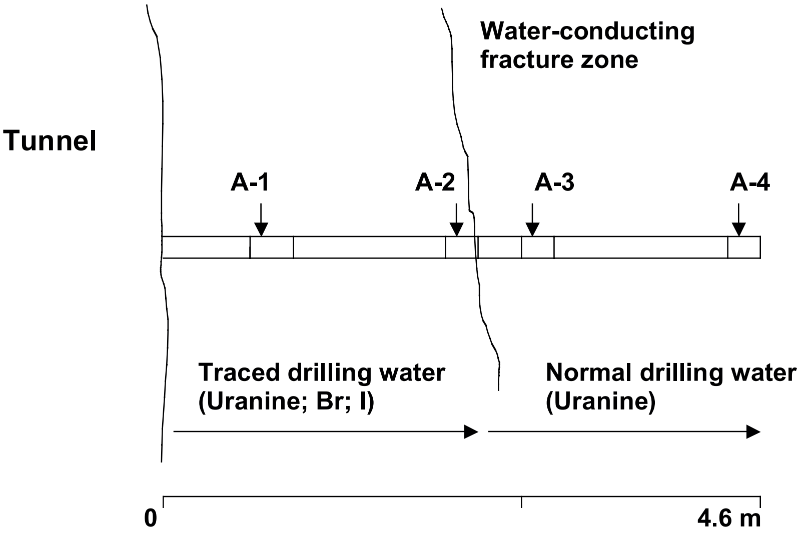

***Figure 3-11.*** *Location of sampled pore waters (A-1 to A-4) from the 420 m level in borehole KA3386A06 at the Äspö HRL.*

Initially, the intention was only to address the potential contamination effects of drilling water as part of the overall PLU investigations. For example, investigate the potential influence of drilling fluid during drilling in a rock no longer affected by stress release, but only by the disturbed zone induced by the drilling process itself. However, rather than miss the opportunity, it was decided to sample also a selected rock profile extending from a water conducting fracture into the adjacent rock matrix, and analyse the extracted pore water for chloride in addition to the added 'contamination' tracers of bromide, iodide and uranine. It was hoped also that a variation in chloride may provide an indication of a chemical gradient close to the water conducting fracture; if so, this change in pore water composition may be related to changes in groundwater compositions in conducting fractures during the Holocene, i.e. since the last deglaciation.

The pore water extraction and analytical approaches were similar to those used in the Forsmark and Laxemar PLU investigations (Waber et al. 2009a, b), and the chloride data therefore are largely comparable. However, this does not mean that data from the initial long term experiment in Borehole KF0051A01were in any way superseded. In fact, these earlier data play an important role in that they have not been subjected to the same potential contamination effects during drilling and extraction of the drillcores, and to uncertainties related to the laboratory extraction and analytical techniques. For example, the long term experiment at Äspö indicates that the matrix pore-waters are less saline than the surrounding fracture groundwaters and do not have a marine component. This supports later findings at Forsmark which at the time were treated with some scepticism surrounding possible contamination during drilling or reflecting laboratory pore-water extraction problems.

### *Available data*

#### Borehole KF0051A01

Based on detailed mineralogical and hydrogeological studies, four borehole sections (S1, S2, S3 and S4) representing microscopically homogeneous unfractured rock matrix of low hydraulic conductivity ($10^{-14}$–$10^{-13}$ $ms^{-1}$), where isolated for long term sampling of *in situ* pore-waters (Figure 3-7). From June 1998 to May 2003 these isolated intervals representing fracture-free zones of texturally and compositionally homogeneous rock matrix were sampled. In May 2003 the borehole packer system was relocated 0.90 m towards the tunnel face to include the small-scale closed microfractures in Sections 3 and 4, while Sections 1 and 2 remained in fracture-free zones. Basically, these relocated samples, especially Sections 3 and 4 which now contain microfractures, may represent 'new' samples, i.e. potentially of varying composition compared to the earlier sampling. This manoeuvre enabled the possibility to relate such effects (i.e. microfractures vs. no microfractures) on the pore-water chemistry. In addition, there was the possibility to compare the pore-water chemistry originating from the two main rock types which characterise the area, i.e. Äspö diorite and Ävrö granite.

The reported sampled data relate, therefore, to pore-waters which accumulated in the isolated drillhole sections under hydrostatic pressure over a 7.5 year period. This was the case for sections S2, S3 and S4 (Figure 3-7) prior to and after relocating the packer system; section S1, with the highest residual volume, had accumulated insufficient porewater and therefore could only be sampled for gas. During the first part of the investigation Sections S2 and S3 were sampled on two occasions and Section S4 on three occasions prior to relocating the packer system. During the second part of the investigation Sections S2, S3 and S4 were sampled on two occasions.

The long term *in situ* reliability of the sampled pore-waters during the experiment varied for sections S2, S3 and S4. Short-term movement of different water types (i.e. during the timescale of the experiment) through some of the rock matrix occurred mainly by small-scale advection via a connecting network of nearby microfractures and by diffusion. Consequently, Section S2 suggests the presence of a younger groundwater component which has accessed the rock matrix during the experiment. However, Sections S3 and S4 represent pore-waters comprising old palaeogroundwaters still preserved in the low hydraulically transmissive rock matrix, although a component of matrix 'pore fluids' (i.e. the water in the pore space of a rock that is only accessible by diffusion) is also present (Waber and Smellie 2008).

Because of the generally small and variable volumes of fluid extracted from the borehole sections, a full analysis was not always possible and certain priorities had to be set following each sampling campaign. Priorities included pH (field and lab), alkalinity, major ions (Na, K, Mg, Ca, Cl and $SO_4$), and some isotopes ($\delta^{18}O$, δD, $^{3}H$, $\delta^{13}C$, $^{14}C$, $^{86}Sr/^{87}Sr$ and ± $^{37}Cl$). Additionally, on some occasions, electric conductivity, temperature and water density were also measured, and dissolved Li, Rb, Cs, Sr, Ba, Mn, $Fe^{2+}$, U, total sulphide, silica, iron and manganese were analysed. Gas analysis, when conducted, included $H_2$, CO, $CO_2$, $CH_4$, $C_2H_4$ and $C_2H_6$. Data for the first stage of the study are available in Smellie et al. (2003); these data, together with the data from the second stage of the study, have been compiled in a separate excel sheet named "MFC-Experiment" in the same excel file as the rest of the previous data (Äspö_Ver4_DataReport.xlsx).

Each borehole section was sampled over a period of 7.5 years but not all parameters were analysed on each occasion. The data corresponding to most of the analysed parameters listed above can be considered reliable. However, there are several parameters that should be treated with caution as they are considered unreliable or suspect for different reasons. These parameters are pH, alkalinity, Mn, Fe(II) and F and the reasons are mainly related to the extensive bacterially mediated sulphate- and iron-reduction processes which perturbed the water composition and altered *in situ* conditions (pH and Eh conditions and, therefore, all related parameters). Unfortunately, with the available borehole water data these perturbations cannot be further quantified.

Based on the measured values for pH and alkalinity, the matrix borehole waters were strongly oversaturated with respect to calcite. The reason for this oversaturation was the coupled processes of sulphate reduction and production of $CO_2$ in the sampling sections, degassing of $CO_2$ and $H_2S$ during sampling, and the fact that substantial amounts of $HS^-$ contributed to the measured total alkalinity. Due to these perturbing effects the pH and carbonate system of the borehole waters could not be adequately corrected and calculated to in-borehole conditions. As a consequence, the saturation states of all other carbonate phases, as well as the $\delta^{13}C$-values of dissolved inorganic carbon, also do not represent in-borehole conditions.

The calculated redox potential was restricted to the second sampling campaign following repositioning of the packer system. Dissolved total sulphur and sulphate were analysed by ICP-AES and IC, respectively. This allowed the amount of sulphur present as dissolved sulphide in the samples to be calculated. Based on this the redox potential was obtained by the sulphide-sulphate couple. As expected from the $H_2S$ smell, all borehole water samples had a reducing redox potential. It should be noted, however, that the calculated redox potential represents minimum values due to the out-gassing of $H_2S$ during sampling. As for Fe(II) contents, amorphous iron hydroxide and goethite were strongly supersaturated at the total iron concentration and pH measured in the laboratory. This is consistent with the change in colour of the water during air exposure and the strongly reducing in-borehole conditions. Under these conditions iron is mainly present as ferrous iron which will become oxidised when in contact with air and precipitate as ferric hydroxides. The presence of iron reducing bacteria in the sampled water further supports the presence of ferrous iron in the borehole sections.

Finally, with respect to fluoride, the reason for the unreliability of the values is related to a contamination problem. Fluorite was strongly oversaturated in all waters sampled in the second campaign due to the very high fluoride concentrations measured in these samples. In crystalline environments fluorite often acts as a solubility control for dissolved fluoride; the oversaturation was thus due to contamination of fluoride from the teflon coating of the steel parts within the packer system.

**Borehole KA3386A06**

In this study the pore-water data originate from four cored borehole lengths sampled at increasing distances from the tunnel wall and also at increased distances from an intercepted single water-conducting fracture in the bedrock (cf. Figure 3.11). These four samples, used for the out-diffusion experiments, consisted of reddish-coloured, hydrothermally altered Äspö diorite, and have water contents and a water-content (connected) porosity that lie in the upper half of the range of other Äspö diorite samples (cf. Smellie et al. 2003).

The extracted porewaters were analysed for $Cl^-$, $Br^-$, $I^-$ and uranine; $Br^-$, $I^-$ and uranine were used as drilling tracers showing that contamination (i.e. along the extent of the chemically disturbed zone into the core sample) from these tracers was minimal, only extending to a maximum of 0.1 mm into the drillcore corresponding to about 0.66% of the total pore volume; this is consistent with a maximum contamination of < 1% derived from tracer mass-balance considerations. This means that the pore-water $Cl^-$ data (between 3,000 and 4,200 mg/L, cf. Waber et al. 2009a) were unaffected by the tracer experiment and therefore can be considered representative.

### 3.2.6 Fracture mineral data

Water/mineral reactions (that may or may not involve biogenic activity) are important for the hydrogechemical understanding and detailed description of the groundwater environment for two main reasons: a) recent water/mineral interaction with the groundwaters influences the present groundwater chemistry and *vice versa* (e.g. dissolution/precipitation of calcite; oxidation/production of pyrite, ion exchange etc), and b) the distribution and chemical/isotopic composition of certain minerals (e.g. calcite, pyrite and Fe-oxyhydroxide) provide information on former physico-chemical conditions which are important for the description and the interpretation of the long-term evolution of the groundwater system. Fracture minerals, and to some extent the adjacent bedrock, participate most actively in water/mineral interaction. Furthermore, fracture minerals may also serve as redox and pH buffers in the case of recharging oxidising groundwaters (e.g. during glaciations and deglaciations).

The fracture mineralogy links also strongly to the geological description of the area by the possibility to use fracture mineralogy for interpretation the low temperature evolution of the bedrock (during the stages of semi-brittle and brittle tectonic regimes, i.e. at least during the last 1.5 Ga in the case of the Laxemar-Äspö area).

The fracture filling data available from Äspö spans over a 25 year period and analytical methods have improved considerably during this period. However, of even greater importance is the use of the triple tube drilling technique which provides much higher quality and better preserved material for sampling and studying fracture fillings (used during the site investigations and during the late drillings at Äspö from about 1999 onwards). Except for the fracture mineral reports related to the pre-investigations (1987–1988; Tullborg 1988), most of the fracture mineral studies up to about year 2000 have concentrated on satisfying the requirements of different experiments. Most of these studies are concentrated on fracture mineral identification in specific structures on a very detailed scale. These include for example: 1) The large scale Redox Experiment (Banwart et al. 1994). 2) The different TRUE experiments, for example the True Block scale (Andersson et al. 2002) or the TRUE-1 Completion (Byegård et al. 2013). 3) The Redox Experiment REX (Puigdomenech et al. 1999) 4) The Matrix Fluid experiment (Smellie et al. 2003). Other projects aimed to develop and improve different methodologies for palaeohydrogeological studies include the EQUIP and Padamot projects running from 1997 to 2005 (Bath et al. 2000, Milodowski et al. 2005).

Overall, the increased knowledge of the sampling methodologies in combination with the increasing amounts of supporting data and improved drillcore quality, resulted in a solid base for the fracture mineralogical studies performed during the site investigations (Tullborg et al. 2008). The fracture mineral studies from Laxemar, being part of the site investigation, are reported in Drake and Tullborg (2009) and numerous P-reports and papers sited in the reports. The fracture mineral results from this site investigation do not only comprise the Laxemar boreholes but also drillcores from Simpevarp and to some extent from Äspö, as well. It is therefore recommended that these reports and the reports and papers referred to therein, should adequately serve as the main references for the fracture mineralogy with the addition, if needed, of relevant detailed information for specific structures from the experiments related to above and new information from the TAS tunnel (ongoing work). The fracture mineral analyses from year 2000 and onwards are stored in Sicada: however, in order to use these data constructively, the background information described in the reports is necessary.

More qualitative information, for example identification of minerals, is of course always more reliable than quantitative analyses. Detailed fracture mineral studies, however, can never provide a sufficient statistical data set to describe, for example, the distribution of minerals which constitute the redox and pH buffers in the system. Therefore, results from drillcore mapping stored in Sicada are essential for these type of interpretations. The method for drillcore mapping has also improved markedly and the method used in the Laxemar site investigations, and now also during the mapping of the boreholes for the TASS tunnel, is much more sophisticated and reliable than previously. For example, downhole imaging of the borehole walls (BIPS) is now used which provides the possibility to obtain orientations of structures etc. For the statistical overview of fracture mineral distribution at Äspö, it will probably be necessary to depend on older mapping which will require caution and careful testing, and most importantly close cooperation with the team responsible for the geological modelling.

Within the two redox experiments carried out at Äspö, i.e. the Large Scale Redox Zone experiment (Banwart et al. 1994), and the REX experiment at a detailed scale (Puigdomenech 1999), the description of the grain sizes of the loose material in the structures became an important issue, and the total amounts of material/fracture surface was also reported for a specific fracture at the REX site.

# 4 Criteria for sample quality classification

## 4.1 General

As described in Section 2.3, the quality or representativity of groundwater samples are influenced by different conditions in the borehole or during the sampling occasion. Furthermore, the quality of the samples in the Äspö dataset is variable and difficult to evaluate since it covers a time period of more than 20 years. During this time both the equipment and the methods employed have undergone development as a result of increased experience and knowledge of groundwater investigations. Despite these modifications, an attempt was made to assess as close as possible the sample quality of the Äspö dataset based on experience from the previous Forsmark, Laxemar and SFR site investigations (Nilsson 2008, Smellie et al. 2008, Smellie and Tullborg 2009, Nilsson et al. 2011). The following aspects were taken into consideration:

- During the pre-investigation phase between 1986 and 1990 several methods for sampling of boreholes drilled from the surface were used (see Tables 2-1 and 2-2): 1) sampling during drilling in borehole sections delimited by a single packer and the bottom of the borehole generally giving samples with high contents of flushing water, 2) sampling during hydraulic testing implying high induced groundwater flow rates and sampling from long borehole sections, 3) sampling using the special mobile chemistry units representing best possible conditions, and 4) monitoring sampling for shorter or longer periods since 1991 to the present time, in boreholes drilled from the surface and the tunnel system with installed fixed packer equipment.
- With respect to hydraulic conditions; flow logging information is absent from many of the Äspö boreholes. However, pressure registrations in adjacent multiple borehole sections allow detection of short circuiting effects during sampling. In fact, regular/continuous pressure monitoring was applied to most of the sampled borehole sections following the pre-investigation phase. The conditions causing unstable groundwater composition could sometimes be identified from these pressure data. A suitable hydraulic effect criterion such as “Pressure responses between sections” was, however, not used in the categorisation since no recent evaluation of the hydrogeological information was available.
- Sampling has been performed both sporadically and for some borehole sections regularly during some longer or shorter periods. These different conditions can affect confidence in the data and this led to the term “sample series” being introduced to denote long term monitoring, while “time series” was used for a short term series of sample collection during continuous discharge of groundwater. Adequate time series and/or sample series are considered important quality criteria. However, depending on the purpose of the investigations even single samples, if satisfactorily based on the rest of criteria, could also be suitable for the characterisation of the system.
- Finally, while the data quality assessment for the datasets from Forsmark and Laxemar could be centred on each borehole section, the quality assessment for the Äspö dataset (and also for the SFR dataset) had to focus on each individual sample due to the very heterogeneous dataset for each borehole section resulting from the varying range of analyses for each sample and the long sampling time spans involved.

## 4.2 Categorisation criteria

When assessing the sample quality category for each borehole section several factors, which can influence the groundwater quality, have to be considered; a) contamination from drilling (e.g. rock flour and drilling water), b) possible impacts caused by sampling conditions (e.g. which techniques are used, how much groundwater should be discharged prior to sampling?, etc), c) analytical performance and integration of data from different sources, and d) the suitability of the coverage for interpretation purposes. Ideally, the classification of groundwater samples into different quality categories should also require evaluation of hydraulic conditions in the borehole, in the section being sampled, and in the surrounding bedrock. However, these were not considered in the Äspö case since no recent evaluation of the hydrogeological information was available and the existing data were patchy and differed in quality.

Several criteria have been taken into account for the categorisation based on what was proposed and used during the Site Investigations in Forsmark, Laxemar and the SFR, with some modifications and additions to comply with the specific case of the Äspö system. These criteria are described in detail below.

The categorisation process will consist of the evaluation of each criterion in each sample and their grading from 1 to 5 depending on their quality. Then, the final category of the sample corresponds to the highest value (lowest quality) given to the criteria.

### 4.2.1 Drilling water content

When evaluating the quality of groundwater samples collected in boreholes drilled from the surface, a major consideration is the potential impact of flushing or drilling water from core drilling on the chemistry of the collected samples. The risk of such contamination is generally much lower when drilling boreholes underground since the flow direction is directed out from the boreholes due to the pressure conditions. However, even underground the occurrence of special situations causing flushing water contamination cannot be completely excluded, for example, due to contact between two adjacent tunnel boreholes. This is the reason why special treatment has been applied to samples taken from the tunnel boreholes, i.e. when there is no information about the drilling water they have automatically been allocated 2 for this criterion.

The choice of the drilling water source is also of great importance because the greater the difference in composition the greater the impact of unwanted contamination. For example, at Äspö it is of special importance to avoid any change in the groundwater marine signature that might impact on the evaluation of the groundwater origin. The strategy for selecting drilling water sources has varied for different boreholes but, generally, groundwater from an adjacent percussion borehole has been used for the drilling of surface boreholes and groundwater from either KA2598A or HD0025A has often been used for the drilling of tunnel boreholes. Furthermore, tap water without Uranine addition has been used in rather large quantities in the HRL for grouting holes, load holes and bolt holes during tunnel excavation (Nilsson G 2012, personal communication). The database Sicada often lacks information on the specific drilling water sources which could have improved the description of expected impacts on the chemistry for the different sampling objects in Chapter 5. Therefore, the gradual decrease in quality for this criterion is assessed only according to the drilling water content.

Historically at SKB, a maximum of 1% drilling water (based on the amount of uranine tracer) has been used to indicate samples of the highest quality; in particular this is relevant for parameters like trace metals, sulphide, TOC/DOC and $^{14}C$ (pmC). The drilling water content limits are ≤ 1% (Category 1), ≤ 5% (Category 2) and ≤ 10% (Category 3). Samples with greater percent of drilling water are excluded for modelling purposes and directly included in Category 5 (see Table 4-1).

### 4.2.2 Charge imbalance

A good charge balance is indicative of a good quality analysis, although it should be complemented with a check of the conductivity values (measured and calculated). A maximum charge imbalance of ±5% is normally accepted for Categories 1 to 4. In the case of very dilute groundwaters (Cl < 60 mg/L) ±10% is also accepted. Samples with greater imbalance are excluded for modelling purposes and directly included in Category 5.

Apart from the charge imbalance calculated by Sicada directly from the analytical results, the charge imbalance after the speciation calculations performed with PHREEQC has also been calculated (Parkhurst and Appelo 1999) for the Äspö groundwaters.

### 4.2.3 Complete sets of analyses

The major ions Na, K, Ca, Mg, Cl, $HCO_3$ and $SO_4$ should be complete for this criterion to be graded as 1 and 2, i.e. it should be possible to calculate a relevant charge balance. The lack of Na, Ca and or Cl (the main ions in these groundwaters) directly allocates a Category 5 to the sample. Contents of the rest of the major elements (i.e. K, Mg, $HCO_3$ and/or $SO_4$) in these waters are much lower and therefore, in the case that one of these is absent, the criterion is graded as 4.

With respect to the minor elements Si, Br, Sr, Li, F, S(II), Fe and Mn, if some of them are missing (even with a complete major element analyses), the criterion will be graded as 2 being suitable for the general hydrogeochemical modelling although not useful for very specific modelling, e.g. redox modelling.

Available $\delta^{18}O$, $\delta^{2}H$, $^{3}H$, $^{14}C$ (pmC) and $\delta^{13}C$ values are necessary for Category 1 as they give an idea of the groundwater origin and the residence time. If there are only data for $\delta^{18}O$, $\delta^{2}H$ and $^{3}H$ the criterion is graded as 2, except in the case where the bicarbonate content is lower than 10 mg/L, when it will still be graded as 1. If only $\delta^{18}O$ and $\delta^{2}H$ are available, this criterion is allocated as 3, and if all these isotopes are missing (or only one remains) the criterion is graded as 4.

### 4.2.4 Time series and sample series data

The possible impacts on analytical quality and sample representativity from different causes may, to some extent, be excluded or verified by other samples from the same borehole section. Available *time series* data, i.e. several samples collected during continuous discharge from the borehole section (days/weeks), is desired in order to prove the stability/representativity of the groundwater composition, or to discover trends during sampling that reveal sampling and representativity problems. This may be an effect of, for example, introduction of shallower groundwater due to pressure gradients.

On the other hand, the long *sample series* of single samples collected more or less regularly during reasonably long periods between 1987 and 2011 are also useful for the quality evaluation of data. Stable water composition or a clear trend in the data would strengthen the reliability of the data, but an unstable or irregular composition during the time period in question does not necessarily reflect poor sampling quality. In systems similar to the SFR or Äspö, the conditions may vary over time due to the external effects of constructing the tunnels.

Where neither time nor sample series are available for the sample, this criterion is considered inadequate and it is graded as 4. However, the composition of the groundwaters sampled prior to the beginning of all the anthropogenic activities could be of great interest to check the original character of the system, even if they have not been sampled on a regular basis. Accordingly, for this group of samples an additional category, Category 3b, has been included. This category is graded as 1 for the charge balance criterion, and as 2 for the drilling water, the completeness of major ions analyses and section lengths. However, the isotopes and/or the sample/time series criteria are graded as 4 (see below).

### 4.2.5 Section lengths

The length of the borehole section being sampled, in combination with the number and position of the flow anomalies present in the section, impact on the sample quality in two aspects. First, it affects the possibilities to resolve the differences in groundwater composition along the borehole. Secondly, the risk that the sample contains a significant contribution of unrepresentative or contaminated water that has remained in the borehole section for some time increases with increasing section length. Since flow logging data are not available from the early boreholes, no plug flow calculations could be performed in order to estimate the discharge volume needed to obtain samples with an insignificant contribution from water remaining in the borehole section.

Only sections lengths lower than 10 metres are graded as 1 and lengths lower than 20 metres are graded as 2. Section lengths > 20 m and > 100 m automatically lower the groundwater quality and in these cases this criterion is graded as 3 and 4, respectively (see Table 4-1). The relevance of this criterion is higher in the cases of short sample or time series (Category 3b) when no other samples can be used to check the stability of the chemistry in the section. Consequently, only very short section lengths (graded as 1 or 2) are accepted for this category.

### 4.2.6 Pressure responses between sections

Most sampling during the time period 1990 to 2011 (after the pre-investigations) have been conducted in borehole sections equipped with fixed packer equipment and pressure sensors for pressure measurements. In these cases, pressure responses may be revealed in adjacent borehole sections during sampling due to connections established via the fracture system in the bedrock (indicated by delayed response) or leakage over the packers (immediate response). The obvious implication for the sample quality is that groundwater representing different borehole sections and flow anomalies are mixed. The information about pressure responses exists and it is possible that the groundwater composition of deviating samples could be explained by looking through these data. However, in the Äspö case the responses were not considered, mainly since no readily available hydrogeological evaluation existed and time and budget constraints did not allow the necessary in-depth study of the extensive hydropressure documentation.

### 4.2.7 Enhanced pH values as an effect of grouting

Single or repeated high pH values in groundwaters have been observed sporadically at several sampling locations in the Äspö HRL and a probable reason is concrete degradation resulting in alkaline plumes when interacting with groundwater. Samples with enhanced pH values due to grouting may be useful for special studies and for the understanding of grouting impacts but should not be used for general modelling purposes. Figure 4-1 displays the distribution of pH values in the Äspö dataset. Most of the 2,020 samples (93.3%) have a pH in the range between pH 7.1 and pH 8.1. Samples with a pH of 8.7 or higher have directly assigned to Category 5 if grouting activities in the borehole or in the close vicinity of the borehole could be verified from the existing documentation. Deviating pH values in the Äspö dataset are discussed in Section 5.1.2 and samples with pH values of 8.7 or higher are listed in Tables 5-1 and 5-2.

## 4.3 Additional factors not considered in the categorisation

Other factors that may affect the sample quality but have been disregarded as quality criteria are:

- Calculated volume of water to be exchanged before sampling (Plug flow calculation) could increase/verify the quality, especially in cases with long section lengths. However, the necessary information to perform the calculations (flow anomalies, transmissivities and positions) are missing for a majority of the boreholes.
- The inclusion of old analyses, prior to the use of ICP AES as a routine procedure (i.e. before 1990), may lower the analytical quality.

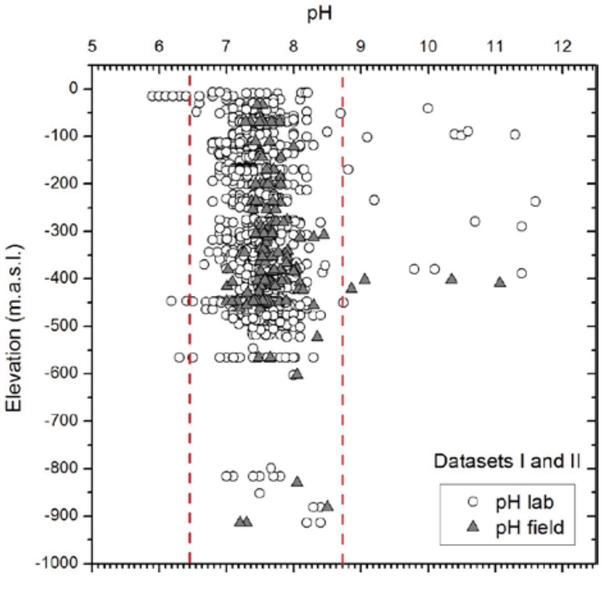

*Figure 4-1.* *pH distribution with depth. There are 2,166 samples with pH values (1,956 lab and 210 field): 17 samples (0.79%) with a pH value between 5.5 and 6.5, 2,126 samples (98.11%) between 6.5 and 8.7, and 22 samples (0.97%) between 8.7 and 12.*

## 4.4 Categorisation process

The categorisation process consists of analysing every sample for all the criteria indicated above (and summarised in Table 4-1) and allocating a suitable category level (grade) to each of them. Then, the final category of the sample as a whole corresponds to the lowest category level given to any of the defined criteria. This means that only Category 1 samples have been graded as 1 for all the criteria. As soon as any of the criteria is evaluated as 2, 3, 4 or 5, the sample will be downgraded to the corresponding level. Generally, there are only a few cases with very good grades in all criteria except for one very low grade. In general, samples tend to have all-pervading good grades or bad grades.

There is a special case, however, that has been taken into consideration in this work due to the importance of having a good characterisation of the system before the tunnel construction: the group of samples representing suitable initial conditions. Some of these samples have very good grades for all the criteria except for the absence of environmental isotopes and/or the absence (or inadequate) sample or time series. The result is that these samples are automatically categorised as Category 4 irrespective of being good quality samples (based on complete major and minor elements, low percent of drilling water and short section lengths) or representing very stable sampling conditions at the surface or underground (which did not require additional sampling, or that additional sampling was not possible; e.g. first strike underground borehole samples considered reliable). Therefore, based on the above, a new Category 3b was defined to include these groundwaters. The explanation of this category together with the others is described next.

Having this in mind, the user must be aware of the fact that a low category (high number) sample could be a good sample from many respects but the lack of information makes the evaluation uncertain. Marking them with a low category assures that any future user will know the possible limitations of these samples although they could be useful for specific situations or studies.

### 4.4.1 Category 1

Samples that are finally categorised as belonging to this group are those that achieved the highest grades for all the criteria, and thereby they are considered the most reliable to characterise the groundwater concerned, including quality input to all kinds of modelling approaches. Following the list of criteria included in Table 4-1: 1) they are the least contaminated by drilling water (content below 1%), 2) they have good quality analyses (good charge balance between ±5%), 3) they show a complete chemical characterisation in terms of all major and minor elements and complete isotopic data, 4) there are adequate sample or time series for the same section, and 5) their section lengths are shorter than 10 m.

### 4.4.2 Category 2

Category 2 samples are the next level in quality and in general they can be used almost for every modelling purpose but should be treated with some caution depending on which criterion (or criteria) has been responsible for a Category 2 qualification. These criteria may include the following: 1) the drilling water content is between 5 and 10% (or there is a lack of information about the drilling water, for example in the case of the tunnel boreholes where it may be assumed to be negligible); 2) their chemical characterisation is incomplete for the minor elements (absence of Br, Fe(II), Mn, Li or Sr) and the $^{14}C$ (pmC) may also be absent, and therefore they cannot be used for specific calculations, correlations or modelling; and 3) the sampled sections are between 10 and 20 m (additional time series and/or sample series would provide more reliability).

### 4.4.3 Category 3

Samples belonging to this group are reasonably good for many purposes but have some limitations to to be taken into account mainly for specific modelling calculations. The amount of drilling water could be as high as 10% and the accepted charge balance is ±5%. This category is also applied when the sample has incomplete environmental isotopes (restricted to $\delta^{18}O$ and $\delta^{2}H$). Finally, the other two possible limitations are related to the inadequate sample series (absence of time series also) and very long section lengths (up to 100 m). As discussed below, except for the fact that these samples have data for $\delta^{18}O$ and $\delta^{2}H$, their overall quality is lower than samples categorised as 3b.

### 4.4.4 Category 3b

This category fulfils the same criteria as Category 1 in the charge balance and as Category 2 in the percent of drilling water, the major and minor components and the section length. However, samples included in this category cannot be considered Category 2 because they neither have environmental isotopes data nor adequate sample or time series. Considering the original categorisation, these samples would have been considered Category 4 and, therefore they would not be used for any additional modelling. However, the fact that they have very good quality analytical data, reasonably short section lengths, and represent the initial conditions of the system, these samples could be used for many modelling purposes except for those that require stable isotope contents. In particular, this category of samples would be very useful to discriminate the groundwater marine component and therefore provide important input to the overall understanding of the site. Figure 4-2 shows the difference in the number of samples suitable for modelling (mainly Category 1 to 3) when considering Category 3b or not. Moreover, as mentioned before, they give an idea of the type of water present initially in the system (in this case water with a clear Littorina signature) that otherwise would be overlooked if the Category 3b samples were not considered.

As this category is only applied to a specific group of samples, those taken before, and early along with, the tunnel construction, it is not included in Table 4-1 with the rest of the categories.

### 4.4.5 Category 4

Samples that are included in this group should not be used for modelling purposes but may still be suitable for the overall site understanding (e.g. groundwater distribution, origin and evolution and its integration with hydrogeology). Depending on which criteria have been graded as 4, their use will have to be cautious. Some of the major elements and most isotopic data may be absent, and/or they could also represent single samples (i.e. no time or sample series) with very long section lengths.

### 4.4.6 Category 5

Groundwater samples included in Category 5 are those which reflect one or more of the following problems:

- incomplete chemical analyses (samples lacking more than one of the major elements),
- high charge imbalances (higher or lower than ±5%),
- high drilling water contents (higher than 10%), and
- high pH values due to grouting activities.

Any of these problems qualifies the sample *sensu stricto* as a Category 5 sample.

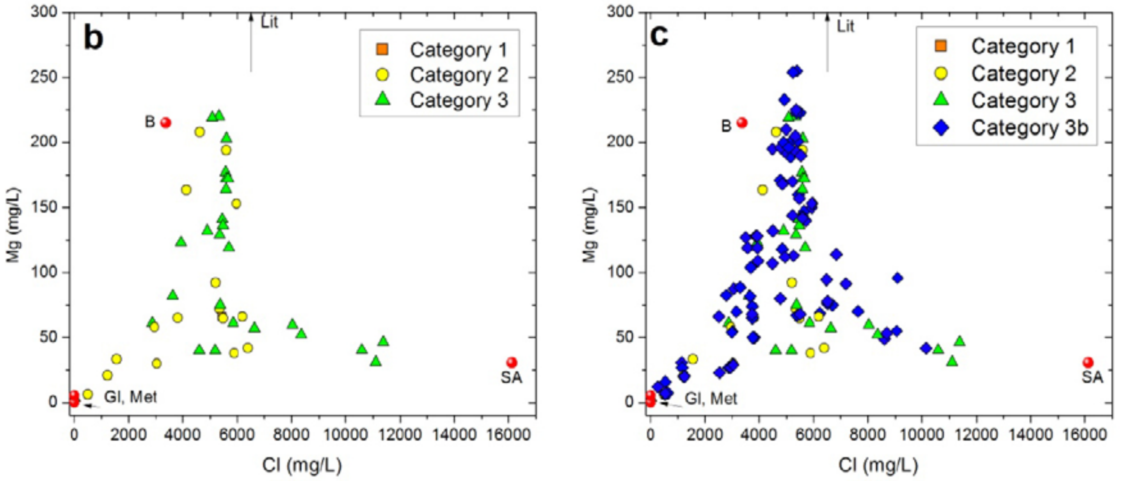

***Figure 4-2.*** *Mg distribution versus Cl in the samples representative of the initial condition in the system. (a) Distribution of the samples belonging to categories 1 to 3. (b) Samples categorised as 3b have been included.*

The data set containing Category 5 samples has been compiled in a separate table in the excel file. They will be considered in the rest of the report only for completion but they should not be used for modelling purposes. However, depending on the study and the samples, they could be used for very specific studies with caution.

**Table 4-1. Categorisation criteria and allocated category number for each criterion. The final category number for each sample corresponds to the lowest grade given to its criteria except for the special case of Category 3b (see text for details). This category is not shown in this general categorisation scheme as it is only applied to the set of samples taken before –, and early along with, the tunnel construction. Samples with more than 10% of drilling water, or with incomplete major ions or with a charge imbalance higher than ±10% are automatically included in Category 5.**

| Criteria | Category | | | | |
|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 |
| **Drilling water** | | | | | |
| (< 1%) | X | | | | |
| (< 5%) | | x | | | |
| (< 10%) | | | x | | |
| (> 10%) | | | | | x |
| Special Case: no information of drilling water from tunnel boreholes | | x | | | |
| **Major and minor components** | | | | | |
| Complete major (Na, K, Ca, Mg, Cl, HCO$^{3}_{-}$, SO$^{4}_{2-}$) and minor ions (Si, Br, Sr, Li, F, S(II) Fe, Mn) | X | | | | |
| Minor ions incomplete: absence of one or more of them. | | x | | | |
| Absence of only one of the following major ions: K, Mg, $HCO_3$, or $SO_4$ | | | | x | |
| Major ions incomplete: absence of more than one of the major elements. | | | | | x |
| **Charge imbalance** | | | | | |
| > ±5% (±10% for < 50 mg/L Cl) | | | | | x |
| Section length | | | | | |
| (< 10 m) | X | | | | |
| (< 20 m) | | x | | | |
| (< 100 m) | | | x | | |
| (> 100 m) | | | | x | |
| **Environmental isotopes** | | | | | |
| Complete: $\delta^{18}O$, $\delta^{2}H$, $^{3}H$, $^{14}C$, $\delta^{13}C$ (except for samples with bicarbonate lower than 10 mg/L where the absence of carbon isotopes is ***** | X | | | | |
| $\delta^{18}O$, $\delta^{2}H$, $^{3}H$ | | x | | | |
| $\delta^{18}O$, $\delta^{2}H$ | | | x | | |
| Incomplete: absence of $\delta^{18}O$ and/or $\delta^{2}H$ | | | | x | |
| **Sample series*** | | | | | |
| Adequate: sufficient number of groundwater samples to be able to trace changes in groundwater composition with time (i.e. months to years) | X | | | | |
| Inadequate | | | x | | |
| **Time series**:** at least three samples collected during continuous pumping or discharge (days or weeks) | X | | | | |
| **Single samples** | | | | x | |

***Sample series** = several separate sampling occasions (annually, each fifth year or weeks to months in between the main occasions). An adequate sample series refers to a sufficient number of groundwater samples to be able to trace changes in groundwater composition with time (i.e. months to years), for example, the gradual transient effects of drawdown due to excavation and construction at the SFR. Availability increases the quality but stability or trends do not influence the quality categorisation.

**** Time series** = at least three samples collected during continuous pumping or discharge from tunnel borehole (duration of days or weeks). An adequate time series refers to a sufficient number of samples to show that the groundwater composition has achieved stability with time (i.e. hours, days to weeks) following drilling and other borehole activities, prior to and during groundwater sampling.

# 5 Sample quality assessment

Among a total of 3,180 hydrochemical samples collected from Äspö during twenty-four years (between 1987 and 2011), there are two groups of samples that have been considered unsuitable for the general modelling. These samples are, however, useful for specific purposes, and therefore, they have not been categorised but stored in separated tables. One group corresponds to the samples taken from weirs (439 samples), which has been stored as Data Set III, and the other is the group of samples collected in the framework of specific projects where the sampling situation may differ in such a way that they can be considered not suitable as representative of the system; (482 samples), which have been compiled as Data Set IV.

So, the quality assessment has been performed over a total of 2,259 samples and this chapter describes the general results. A general description of the criteria evaluation in the whole set of samples is shown first. Then there is a summary of the categorisation results in terms of number of samples in the different categories and the quality of the samples over time or associated with different projects. And finally a series of consistency checks performed in order to give strength to the data quality presented.

## 5.1 General evaluation of the categorisation criteria

This section presents the general results obtained for the different categorisation criteria for samples in Data Sets I and II making a special description of the calculated charge imbalance, the cases of high pH values affected by grouting and the sample and time series. This analysis gives a good idea of the general quality of the studied groundwater data set.

### 5.1.1 Charge imbalance

The charge imbalance (CI) used here has been calculated by PHREEQC from speciation over all the samples from Data Sets I and II with complete major ions, that is 1,713 samples in total.

Figure 5-1 shows the frequency histograms with the number and percent of samples (a and b, respectively) whose charge balance is in a specific range of values (bars in this case representing a range of 0.2%). The information obtained from these plots can be summarised as follows:

- 6 samples (0.35%) with a charge imbalance between –18 and –10%,
- 38 samples (2.74%) between –10 and –5%,
- 1,650 (96.3%) samples between –5 and +5%,
- 9 samples (0.53%) between +5 and +10% and
- 1 (0.06%) between +10% and +12%.

Samples from Categories 1 to 4 all have charge imbalance values inside the ±5% range (indicated with two red discontinuous lines enclosing the majority of the samples). These results were almost identical to the ones obtained by using the WATEQ4F code (Ball and Nordstrom 2001) to calculate the charge imbalance (very good correlation between both results: $r^2=0.95$).

### 5.1.2 Deviating pH values

The distribution of pH values measured (laboratory and field) in the samples from Data Sets I and II is presented in Figures 5-2 and 5-3. Most of the pH values are distributed in the pH range between 6.5 and 8.7 which is indicated in the plots with two red discontinuous lines enclosing the compact block of data points.

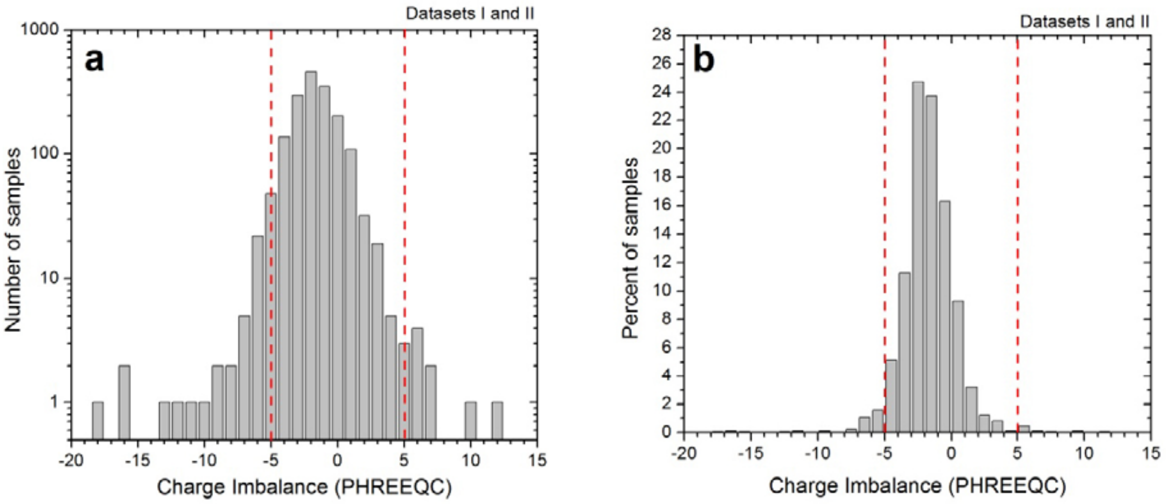

***Figure 5-1.*** *Number of samples (a) and percent (b) with a specific charge imbalance (calculated from speciation by PHREEQC).*

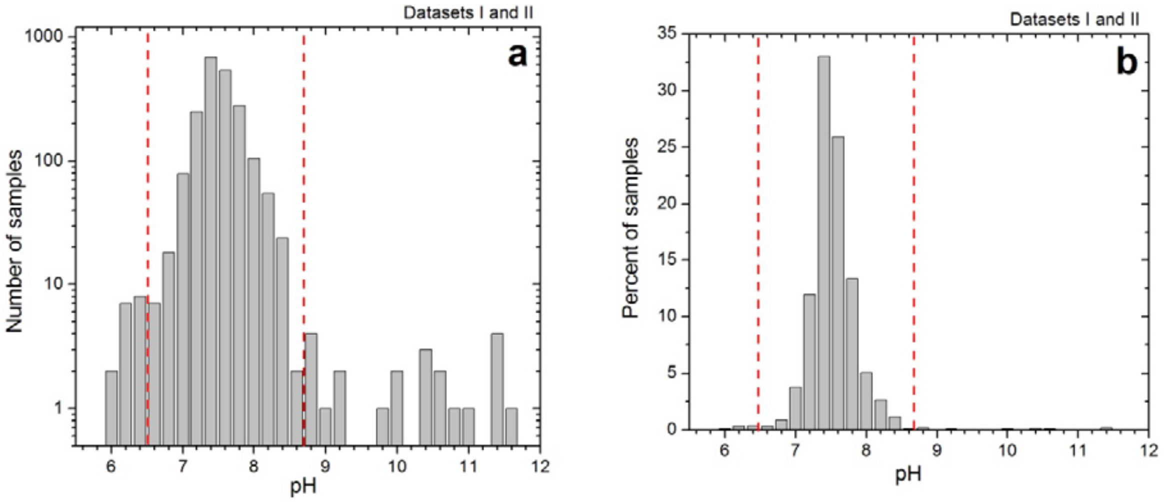

***Figure 5-2.*** *Number of samples (a) and percent (b) with a specific pH value (laboratory and field measurements are considered here).*

There are 2,084 samples with measured pH values (1,876 lab and 208 field) which distribute in the following ranges shown in Figure 5-4: 17 samples (0.82%) with a pH value between 5.5 and 6.5 (only 1 lower that 6, 5.9), 2,045 samples (98%) between 6.5 and 8.7, and 22 samples (1.1%) between 8.7 and 12. Looking in detail, most of the samples (1,755, 84%) have a pH in the range between pH 7.3 and pH 7.9.

Considering this pH distribution in the system, samples with a pH of 8.7 or higher have been directly assigned to Category 5 if grouting activities in the borehole or in the close vicinity of the borehole could be verified from the existing documentation (see Section 4.2.7). Samples with pH values of 8.7 or higher are listed in Table 5-1 and the probable causes for these values are indicated. Most of these samples were collected shortly after grout injection in the borehole or adjacent to the borehole according to the documentation listed below in Table 5-2.

Due to the importance of knowing the effects of grouting on the chemistry of the groundwater system, the same kind of analyses have also been performed on the group of samples from weirs, from the surface points and from the tunnel floor, and the results are presented in Table 5-2.

With respect to the pH distribution with depth, Figure 5-3 shows the absence of a clear trend and the range of pH values is similar at all depths. This is also valid irrespective of the measurement having been carried out in the laboratory or in the field as it was shown in Section 4.2.7 (Figure 4-1), and irrespective of the final category of the samples.

**Table 5-1. Observations of high pH values (pH ≥ 8.7) in boreholes in the Äspö dataset and suggested causes.**

| Idcode | Date | Secup (m) | Seclow (m) | pHl/ pHf | Sample no (Data Set) | Suggested causes |
|---|---|---|---|---|---|---|
| HA1290F | 1992-03-24 | 0.00 | 10.00 | 10.30 | 13300 (DSII) | Grouting of tunnel roof at 1,290 m tunnel length 1992-03-23 and grouting of tunnel face at 1,289.9 m tunnel length, regrouting of various holes 1992-03-24[1]. |
| KA2048B | 1993-02-07 | 0.00 | 45.80 | 10.70 | 13756 (DSII) | The borehole is grouted 1993-02-08 from 0 to 45.8 m borehole length. Incomplete analyses[1]. One of the dates may be erroneous[1]. |
| KA2861A | 1999-02-18 | 8.69 | 9.34 | 9.80 | 2831 (DSII) | The Rex project[2]. Sample collected from the reaction loop. Increase of pH was observed after injection of oxygen. |
| KA2861A | 1999-05-19 | 8.69 | 9.34 | 10.10 | 2925 (DSII) | The Rex project[2]. Sample collected from the reaction loop. Increase of pH was observed after injection of oxygen. |
| KA3007A01 | 2011-04-27 | 0.00 | 13.22 | 10.00/ 10.35 | 20667 (DSII) | Several sections sampled during drilling. The borehole interval 3.9–12.36 m was grouted in 2011-04-18[4]. |
| KA3007A01 | 2011-04-27 | 0.00 | 16.78 | 8.34/ 9.06 | 20666 (DSII) | Several sections sampled during drilling. The borehole interval 3.9–12.36 m was grouted in 2011-04-18[4]. |
| KA3007A01 | 2011-05-09 | 0.00 | 72.68 | 10.00/ 11.07 | 20670 (DSII) | Several sections sampled during drilling. The borehole interval 12. 0–17.0 m was grouted in 2011-05-06[4]. |
| KA3007A01 | 2011-05-12 | 0.00 | 166.78 | 9.97/ 8.86 | 20672 (DSII) | Several sections sampled during drilling. The borehole interval 12. 0–17.0 m was grouted in 2011-05-06[4]. |
| KI0023B | 1997-10-23 | 5.91 | 8.79 | 8.74 | 2464 (DSII) | Sampling just after drilling. No information about grouting. |
| KXBLOTS1 | 1996-10-10 | 0.00 | 5.78 | 9.70 | 2364 (DSIV) | Induced high pH from cement. |
| SA0289A | 1991-02-19 | 6.00 | 19.90 | 10.00 | 13169 (DSIV) | Sampled just after percussion drilling during tunnel construction. Grouting was performed at 275.9 and 284.5 m tunnel length in 1991-01-08 and 1991-01-11[1]. |
| SA0361B | 1991-02-12 | 6.00 | 19.00 | 8.70 | 13165 (DSII) | Sampled just after percussion drilling during tunnel construction. Grouting was performed at 284.5 m tunnel length in 1991-01-11[1]. |
| SA1713A | 1992-10-22 | 5.80 | 20.10 | 9.20 | 76 (DSII) | Sampled just after percussion drilling during tunnel construction. Grouting at 1,693 m tunnel length in 1992-10-20 (connection, surface leakage). After-grouting later on[1]. |
| SA1730A | 1992-10-29 | 5.60 | 20.00 | 11.60 | 13720 (DSII) | Sampled just after percussion drilling during tunnel construction. Grouting at 1,725.8 m tunnel length in 1992-10-28 (connection + sonde borehole)[1]. Incomplete major ions. |
| SA2142B | 1993-02-23 | 6.00 | 20.40 | 11.40 | 59 (DSII) | Sampled just after percussion drilling during tunnel construction. Grouting at 2,141.9 m tunnel length in 1993-02-22 (connection)[1]. |
| SA2912A | 1994-02-04 | 0.00 | 20.00 | 11.40 | 13900 (DSII) | Sampled just after percussion drilling during tunnel construction. Grouting at 2,912.0 m tunnel length in 1994-02-03 (connection)[1]. |
| SS0032A02 | 2008-05-22 | 0.00 | 20.00 | 11.00 | 14532 (DSIV) | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fume[5]. |

* Explanations to superscripts below in Table 5-2.

**Table 5-2. Observations and suggested causes in the Äspö dataset of high pH values (pH ≥ 8.7) measured in weirs, surface sampling points and from sampling the tunnel floor.**

| Idcode | Date | Secup (m) | Seclow (m) | pH_L* | Sample no. (Data Set) | Suggested causes |
|---|---|---|---|---|---|---|
| MA2840G | 1999-04-06 | | | 8.90 | 2852 | Following grouting in 1995-05-21, weir cleaning in 1998 and weir calibration in 1999-02-10[1]. |
| MA3426G | 2007-12-07 | | | 8.96 | 14466 | Cleaning using Silicasol in 2007-11-29; disturbance from project SU32516 Fintätning[1]. |
| MA3426G | 2008-09-15 | | | 9.25 | 14623 | The disturbance seems to remain; see above[1]. |
| PA2013F | 1993-01-13 | | | 11.70 | 13746 | (YA2013F), sampling location in tunnel front during tunnel construction. Grouting at 2,013.2 m borehole length in 1993-01-14. One of the dates may be erroneous[1]. |
| TASS | 2008-04-17 | 20.00 | 20.00 | 9.01 | 14511 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |
| TASS | 2008-06-04 | 21.00 | 21.00 | 8.94 | 14540 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |
| TASS | 2008-06-17 | 22.00 | 22.00 | 9.27 | 14544 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |
| TASS | 2008-06-10 | 23.00 | 23.00 | 9.37 | 14542 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |
| TASS | 2008-06-05 | 35.00 | 35.00 | 10.00 | 14541 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |
| TASS | 2008-06-12 | 43.00 | 43.00 | 8.90 | 14543 | SU32516 Fintätning. Test of grouting technique during construction of a short tunnel (TASS). Use of grout with low pH and silica fumes[5]. Sampling from tunnel floor. |

[1] Sicada/activity log and Sicada/activity comment.

[2] REX.

[3] LOTS.

[4] Projecting of the tunnels TASP and TASU as well as adjacent niches.

[5] Funehag 2008.

pH_L = laboratory value.

Deviating low pH values (i.e. outside the left frame limit in Figures 5-2 and 5-3) correspond to:

1) Fourteen samples at shallow depths (at around –15 m depth) from the same section in borehole HBH02. These low pH values are probably representative and due to a large contribution of recent meteoric precipitation to the groundwater.

2) Three samples at around –447 m depth from three different boreholes. The boreholes are KA3386A (#14405; GWCM), KA3548A01 (#2574; Prototype) and KF0051A01/1 (#3988; Matrix). These borehole sections have additional samples from regular sampling during many years and these other samples show pH values in the expected range. The low pH values may be due to erroneous measurements or impacts from experiments and activities in the HRL. Contamination with tap water or acid fumes from residual acid in sample bottles prepared in advance is possible causes.

3) Two samples at –566.28 m depth. The two samples were collected in 1991 and 1997 from a monitored borehole section in borehole KAS03 and have the lowest pH values in a series of samples with a large variation in water composition as well as pH (pH variation between 6.3 and 8).

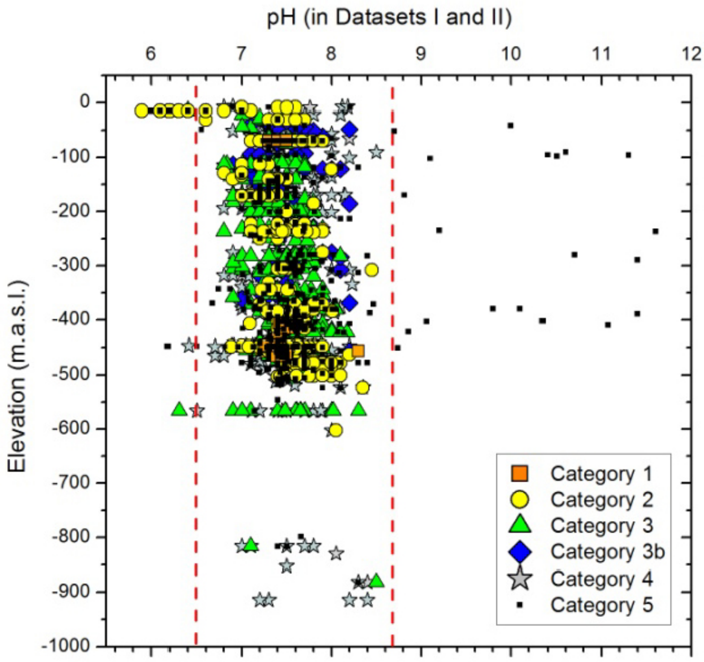

***Figure 5-3.** pH distribution with depth in samples from Data Sets I and II. Samples are coloured coded and plotted with a different symbol as a function of their category.*

### 5.1.3 Sample and time series

A general description of the number of boreholes (included in Data Sets I and II) with more or less adequate samples and/or time series is presented in this section. They have been separated in several groups to facilitate their description and to emphasise their suitability for future modelling: a) boreholes with only single samples, b) boreholes with 2, 3 or 4 samples, and c) boreholes with more than 4 samples.

**Data Set I (195 tunnel boreholes):**

- Only *single samples*: there are 74 boreholes with only one sample and 57 of them correspond to Initial Conditions. There are 23 additional samples associated with some of these boreholes that are included in Category 5 (implying that in some cases they had more than one sample but only one has been considered acceptable) mainly due to the incomplete major elements.
- Series (either sample or time series) of *2, 3 and 4 samples*: there are 23 boreholes with two samples, 15 with 3 and 14 with 4 samples in DS I, that is, a total of 147 samples from which 30 samples correspond to Initial Conditions. Another 75 additional samples associated with some of these boreholes are included in Category 5, again due to incomplete major elements but also 28 of them correspond to the Äspö Extension Project.
- Series (either sample or time series) with *more than 4 samples*: there are 69 boreholes with more than 4 samples which give a total of 989 samples of Categories 1 to 4 and in general show a lower category number than the other groups. Only 37 of these samples have been considered representative of the Initial Conditions. Another 372 additional samples associated with some of these boreholes are included in Category 5 (321 of them due to incomplete major ions).

**Data Set I (27 surface boreholes):** All of them have adequate time or sample series with more than 4 samples. The total amount of samples is 375 from which 138 are considered representative of the Initial Conditions. There are 58 Category 5 samples associated with some of these boreholes which have incomplete major ions and unacceptable charge imbalance.

**Data Set II (58 boreholes without samples in Data Set I):** Most of these boreholes were associated with the tunnel construction (0–750 and 750–3,191 m) and many of them (those with the highest number of samples) are probing boreholes. The number of boreholes in each group is:

a) Only single samples: 44 boreholes (44 samples).

b) Series of 2 and 3 samples: 7 boreholes (16 samples).

c) Series with more than 4 samples: 7 boreholes (91 samples).

A summary of the number of samples fulfilling the series criteria are shown in Figure 5-4b.

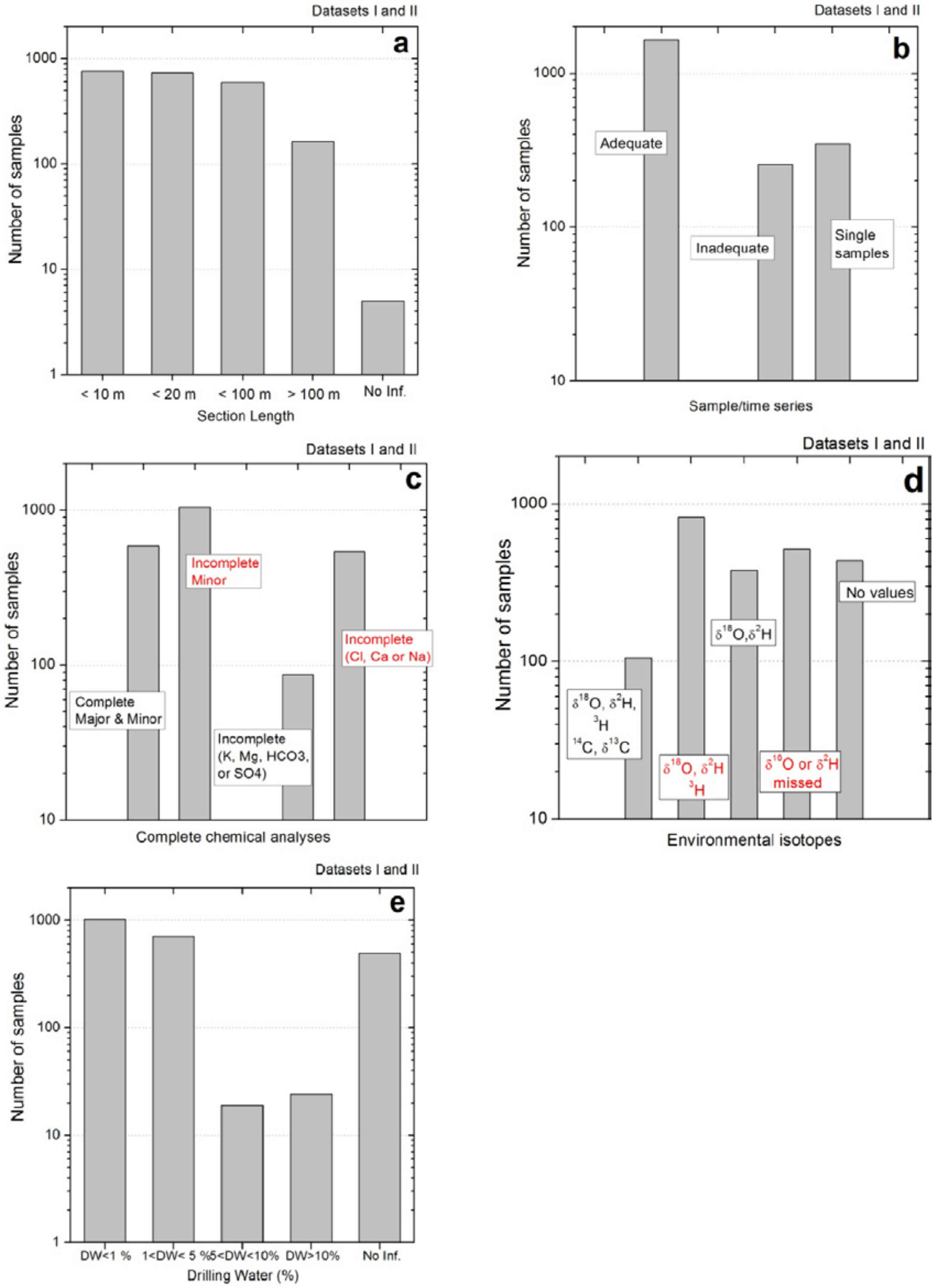

***Figure 5-4.** Categorisation criteria and number of samples for each criteria.*

### 5.1.4 Other criteria

The grading of the rest of the criteria used for the categorisation of the samples is shown in Figure 5-4. For each criteria the number of samples which accomplish a specific value in the criteria ranges is indicated.

As shown in Figure 5-4a, there is almost the same number of samples with sections less than 10 metres long (760 samples), than with section lengths between 10 and 20 m (738 samples) and they have been graded as 1 and 2 respectively for this criteria. Then there are 593 samples with section lengths between 20 m and 100 m, and the grade for this criterion is 3, and 163 samples with lengths longer than 100 m, which have been graded as 4 for this criterion.

Figure 5-4b shows the number of samples with adequate or inadequate sample or time series and the number of samples with adequate sampling series is 1,656 compared to the 255 samples with inadequate series and 348 single samples.

Figure 5-4c shows that the number of samples with complete chemical analyses for the major ions is very important, 1,628, although 1,040 do not have complete minor ion data. Another 87 samples have complete major ions analyses except for K, Mg, $HCO_3$ and/or $SO_4$. Finally, there are 544 samples without data for Cl, Ca and/or Na (Category 5 samples).

The situation with the isotopes is different as there are relatively few samples with complete information on the environmental isotopes (105 samples; Figure 5-4d) while 436 samples do not have any isotopic data. This is generally a consequence of the common strategy to select only a few samples from a time series for isotope determinations. 823 samples have been analysed for $^{18}$O, $^{2}$H and $^{3}$H but not for the carbon isotopes, 379 contain data only for $^{18}$O and $^{2}$H, and finally 516 only have data for one isotope.

Figure 5-4e shows the drilling water criteria. 1,723 samples have a low percent of drilling water, 1,018 lower than 1 (the criteria has been graded with 1) and 705 lower than 5% (criteria graded with 2). There are around 500 samples without information regarding the percent of drilling water but most of them correspond to tunnel boreholes where the presence of drilling water is considered negligible; in these cases the criteria is also graded with 2. The number of samples with a high percent of drilling water is very low, 19 of them have between 5 and 10 percent, and in 24 samples the percent is higher than 10 (Category 5).

Once the different categorisation criteria were assessed and graded for all the samples, they were categorised according to the lowest grade (highest number) given to its criteria (except the special case of Category 3b, see Chapter 4).

## 5.2 General results

From the total of samples categorised (2,259), 1,585 have been evaluated as belonging to Categories 1 to 4 and they are included in Data Set I (375 correspond to surface boreholes and 1,210 to tunnel boreholes). 674 samples were judged as Category 5 and are included in Dataset II (71 correspond to surface boreholes and 603 to tunnel boreholes).

### 5.2.1 Date Set I: Categories 1 to 4

Figure 5-5 summarises the general results obtained for each year as a result of the categorisation indicating the number of samples belonging to quality Categories 1 to 4. Even though the sample quality assessment is not a straightforward procedure, this categorisation as presented in Figure 5-3 provides a good general idea of the quality of the Äspö dataset.

The number of samples belonging to Category 1 is quite small (29) and represents only 1.83% of the total number of samples. Categories 2 and 3 contain almost the same number of samples each, 453 (28.6%) and 418 (26.4%), respectively. There are 583 (36.8%) samples qualified as Category 4 and another 102 (6.4%) that have been included in the new Category 3b. Considering the heterogeneity of the sampling conditions, there are plenty of useful and reliable data available for modelling of the Äspö groundwater system. The evolution in the quality of the data with time, expressed as a higher amount of samples belonging to better categories, is presented in Figure 5-5 and Table 5-3. The quality of the samples taken in the framework of each project is also shown in Figure 5-5 and is summarised in Table 5-4.

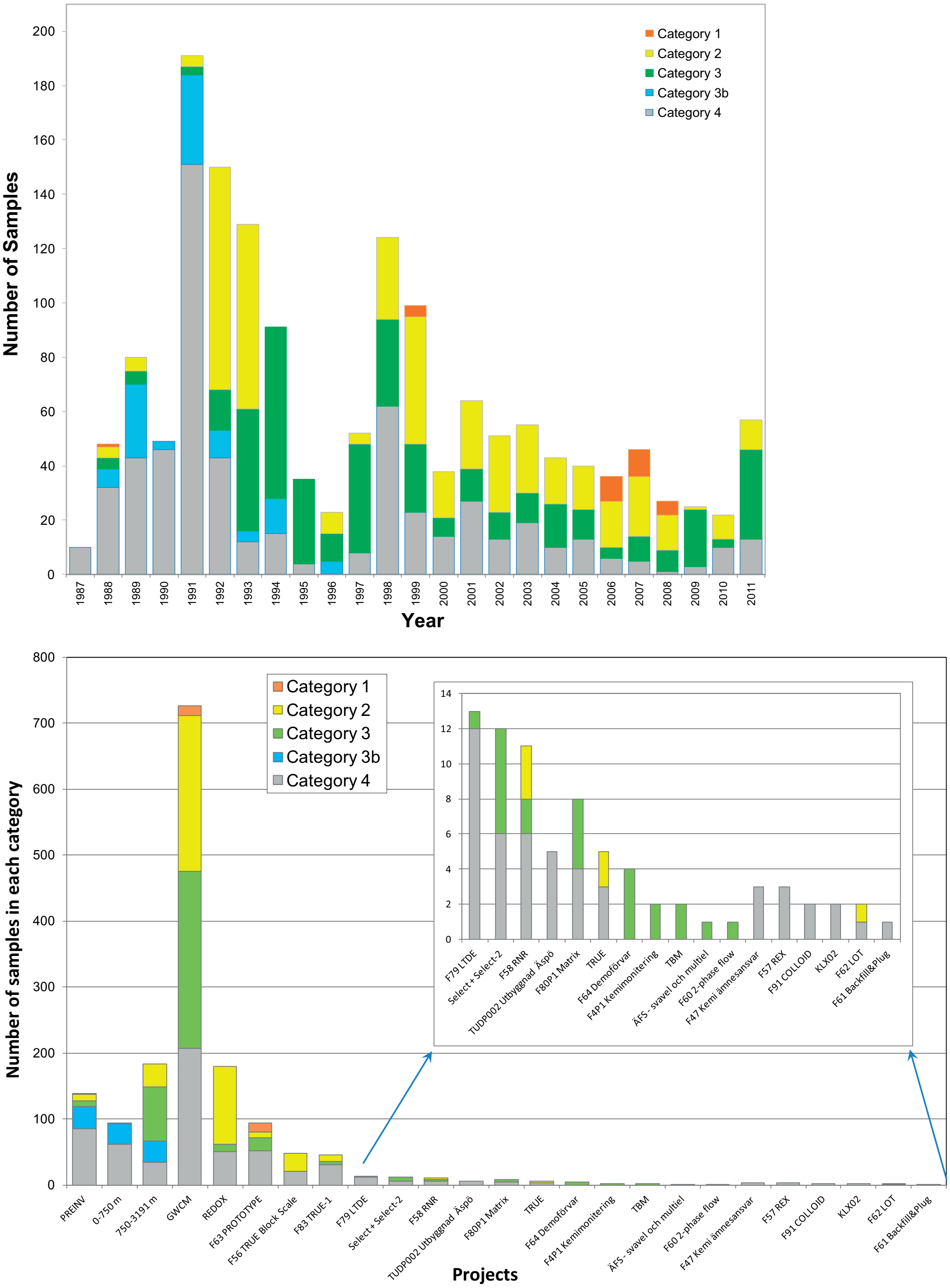

*Figure 5-5. Number of samples categorised as 1, 2, 3, 3b and 4 for each year (above) and project (below) during the time period 1987 to 2011.*

**Table 5-3. Number of samples corresponding to Categories 1, 2, 3, 3b and 4 during the period 1987–2011. In this and the following table, the column "Comments" gives a short description of the quality of the samples indicating the reasons why the samples have been categorised as indicated. The last column indicates the projects and the number of samples taken associated with them.**

| | | Number of samples in each category | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Year** | **Total** | **1** | **2** | **3** | **3b** | **4** | **Comments** | **Projects ongoing during the year with samples taken (in brackets)** |
| 1987 | 10 | | | | | 10 | Absence of time or sample series and very long section lengths (20 to 100 m). | Pre-investigation (10) |
| 1988 | 48 | 1 | 4 | 4 | 7 | 32 | Cats 3, 3b and 4 due to the lack of isotopes, incomplete major ions and some very long section lengths (> 100 m) | Pre-investigation (48) |
| 1989 | 80 | | 5 | 5 | 27 | 43 | Cats 3, 3b and 4 due to the lack of isotopes, incomplete major ions and some very long section lengths (> 100 m). High number of Cat 3b samples. | Pre-investigation (80) |
| 1990 | 49 | | | | 3 | 46 | Cats 3b and 4 due to the lack of isotopes mainly, some very long section lengths (20 to 100 m) and some incomplete major ions. The tunnel construction and the monitoring programme started. | 0–750 m (5)<br>GWCM (44) |
| 1991 | 191 | | 4 | 3 | 33 | 151 | Year with the maximum number of samples taken (mainly associated with the tunnel construction, then the monitoring and the Redox project). High number of Cat. 3b samples, good quality but no isotopes. Cat 4 mainly due to the lack of isotopes and long sections. | 0–750 m (87) / 750–3,191 m (12)<br>GWCM (53) / Redox (39) |
| 1992 | 150 | | 82 | 15 | 10 | 43 | High number of samples taken (from the Redox project and associated with the tunnel construction). Highest percent of Cat 2, more than the other categories together (from the Redox project). Cat 4 mainly due to the lack of isotopes, long sections and absence of time or samples series. | 0–750 m (1) / 750–3,191 m (43)<br>GWCM (18) / Redox (88) |
| 1993 | 129 | | 68 | 45 | 4 | 12 | High number of samples (tunnel construction and Redox project). High percent of Cat. 2 and 3 and very few low category samples. Cat 4 mainly due to the absence of time or samples series and the long sections. | 750–3,191 m (72) / KLX02 (2)<br>GWCM (10) / Redox (45) |
| 1994 | 91 | | | 63 | 13 | 15 | Highest number of Cat 3 samples, with reasonably good quality (including time and samples series but incomplete isotopes). Cat 4 mainly due to the lack of isotopes and long sections (from the GWCM). End of the tunnel construction. | 0–750 m (1) / 750–3,191 m (56)<br>GWCM (18) / Redox (8) / Select (5)<br>TBM (2) / F60 2-phase flow (1) |
| 1995 | 35 | | | 31 | | 4 | Low number of samples. High number of cat 3, with reasonable good quality (including time and samples series) except for incomplete isotopes. | GWCM (27) / Select (6) / F58 RNR (2) |
| 1996 | 23 | | 8 | 10 | | 5 | Low number of samples. Good quality samples: 80% correspond to Categories 2 and 3. Category 4 samples due to the inadequate time or sample series. They correspond to the F83 TRUE-1 + TRUE project. | GWCM (13) / F83 TRUE-1 + TRUE (9)<br>F64 Demoförvar (1) |
| 1997 | 52 | | 4 | 40 | | 8 | High number of Cat. 3 samples compared with the other categories. Cat. 4 due to the incomplete isotopes and long sections. They correspond to the monitoring programme (GWCM) | GWCM (47) / F83 TRUE-1 + TRUE (2)<br>F64 Demoförvar (3) |
| 1998 | 124 | | 30 | 32 | | 62 | High number of samples (from GWCM and Prototype project). Variable quality, half correspond to Categories 2 and 3 and the other half to Cat. 4 (inadequate time or sample series and incomplete isotopes and major ions; Prototype). | GWCM (70) / F83 TRUE-1 + TRUE (1)<br>F56 TRUE Block Scale (1)<br>F63 Prototype (49) / F57 REX (3) |

| Year | Total | Number of samples in each category | | | | | Comments | Projects ongoing during the year with samples taken (in brackets) |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | | |
| 1999 | 99 | 4 | 47 | 25 | | 23 | Relatively high number of samples (from GWCM). 4 samples belong to Cat 1 (GWCM). Cats. 2 and 3 correspond to samples taken in F56 TRUE Block Scale and GWCM. The main reason for Cat. 4 samples is the inadequate time or sample series and the long sections. | GWCM (72) / F63 Prototype (3)<br>F56 TRUE Block Scale (16) / Select (1)<br>F58 RNR (5) / F80P1 Matrix (1)<br>F61 Backfill & Plug (1) |
| 2000 | 38 | | 17 | 7 | | 14 | Low number of samples. Cat. 4 samples due to the lack of time or samples series (mainly) and to the long sections. | GWCM (23) / F83 TRUE-1 + TRUE (1)<br>F56 TRUE Block Scale (10) / F58 RNR (2) / F79 LTDE (1) / F62 LOT (1) |
| 2001 | 64 | | 25 | 12 | | 27 | In general, samples from GWCM are better quality than samples from F83 TRUE-1 + TRUE. Cat. 4 samples mainly due to incomplete isotopes. | GWCM (34) / F80P1 Matrix (3)<br>F83 TRUE-1 + TRUE (27) |
| 2002 | 51 | | 28 | 10 | | 13 | Reasonably good quality in general. The few samples that belong to Cat 4 come mainly from the F56 TRUE Block Scale and the category has been given due to the lack of time or sample series (mainly) and the length of the sections. | GWCM (30)<br>F56 TRUE Block Scale (21) |
| 2003 | 55 | | 25 | 11 | | 19 | Cat. 2 and 3 samples come from GWCM. Cat. 4 is mainly due to the lack of complete major ions and isotopes and they come mainly from F79 LTDE. | GWCM (32) / F83 TRUE-1 + TRUE (5)<br>F80P1 Matrix (4) / F58 RNR (2)<br>F63 Prototype (2) / F79 LTDE (10) |
| 2004 | 43 | | 17 | 16 | | 10 | Reasonably good samples. Cat. 4 due to the inadequate time and sample series. | GWCM (27) / F83 TRUE-1 + TRUE (5)<br>F79 LTDE (1) / F63 Prototype (9)<br>ÄFS – svavel och multielement (1) |
| 2005 | 40 | | 16 | 11 | | 13 | Samples from Categories 2 and 3 come from GWCM. Cat, 4 due to the incomplete time and sample series. | GWCM (37)<br>F47 Kemi ämnesansvar (3) |
| 2006 | 36 | 9 | 17 | 4 | | 6 | Low number of samples but 9 of them belong to Cat. 1 (Prototype). Cats 2 and 3 cover almost all the rest of the samples and come mainly from the GWCM. Only 6 samples are included in Cat. 4 (from F91 Colloid, and GWCM) due to the long sections and the lack of isotopes. | GWCM (20) / F79 LTDE (1)<br>F63 Prototype (12)<br>F62 LOT (1) / F91 COLLOID (2) |
| 2007 | 46 | 10 | 22 | 9 | | 5 | 10 samples belong to Cat. 1. Only 5 Cat, 4 samples because of the incomplete isotopes. | GWCM (36)<br>F63 Prototype (10) |
| 2008 | 27 | 5 | 13 | 8 | | 1 | 5 samples of Cat. 1. Only one sample of low category. | GWCM (27) |
| 2009 | 25 | | 1 | 21 | | 3 | Samples mainly from Cat. 3, due to the incomplete isotopes. Cat, 4 samples (only 3) also show incomplete isotopes or long sections. | GWCM (24) / F63 Prototype (1) |
| 2010 | 22 | | 9 | 3 | | 10 | The lowest quality ones come from KBP1001 'Brytning av prototypförvaret' and the reason why they are Cat. 4 is due to the lack of isotopes. | GWCM (14) / KBP1001 Brytning av prototypförvaret (8) |
| 2011 | 57 | | 11 | 33 | | 13 | Samples from Categories 2 and 3 come from the GWCM. Low quality samples correspond mainly to the 'TUDP002 Utbyggnad Äspö'. Category 4 due to the inadequate time or sample series and /or due to the long sections. | GWCM (50) / F4P1 Kemimonitering (2)<br>TUDP002 Utbyggnad Äspö (5) |

**Table 5-4. Number of samples included in Categories 1, 2, 3, 3b and 4 (Data Set I) associated with the different projects.**

| Project | Tot no. | Categories and number of samples | | | | | Comments |
|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | |
| PREINV | 140 | 1 | 9 | 9 | 34 | 87 | Not very good quality for the incomplete isotope data (transformed in Category 3b).<br>Cat 4: some very long sections, incomplete isotopes, some incomplete ions and some single samples. |
| 0–750 m | 94 | | | 2 | 31 | 61 | Not very good quality in general, only 2 Cat. 3 samples. Cat 3b: incomplete isotopes and inadequate monitoring series. Cat 4: incomplete isotopes, long sections and inadequate series. |
| 750–3,191 m | 183 | | 35 | 82 | 32 | 34 | Cat 3: incomplete isotopes mainly, some inadequate series and some long sections. Cat 3b: many single samples and incomplete isotopes. Cat 4: mainly due to the long sections (apart from incomplete isotopes and single samples or inadequate time or sample series). |
| GWCM | 726 | 14 | 237 | 268 | | 207 | Good quality in general. Cat 3 due to the long sections and the incomplete isotopes data. Cat 4 due mainly to the long sections and incomplete isotopes, and some samples with incomplete major ions. |
| Redox | 180 | | 119 | 11 | | 50 | Very good quality. Cat 4 only because of the incomplete isotopes data, very good for the rest of criteria in many cases. |
| F63 Prototype | 94 | 14 | 9 | 19 | | 52 | Very good quality in general. Cat 4: single samples or inadequate series mainly, incomplete isotopes and some long sections. |
| F56 TRUE Block Scale | 48 | | 28 | | | 20 | Good quality in general except for some single samples (Cat 3b, 4) and length of the sections (Cat 4). |
| F83 TRUE-1 | 45 | | 10 | 4 | | 31 | Reasonably good quality in general except in Cat 4 for the incomplete isotopes data and single samples. |
| F79 LTDE | 13 | | | 1 | | 12 | Low category samples mainly due to the incomplete major ions apart from the incomplete isotopes. |
| Select + Select-2 | 12 | | | 6 | | 6 | Single samples or inadequate monitoring series, incomplete isotopes and some long sections. |
| F58 RNR | 11 | | 3 | 2 | | 6 | Reasonably good quality except some of them have incomplete isotopes or single samples with long sections |
| F80P1 Matrix | 8 | | | 4 | | 4 | Cat. 3 mainly due to inadequate series. Cat 4 due to incomplete major ions and isotopes. |
| TRUE | 5 | | 2 | | | 3 | Single samples, one with a long section. |
| F47 Kemi ämnesansvar | 3 | | | | | 3 | All single samples with long sections. |
| F57 REX | 3 | | | | | 3 | Incomplete isotopes but rest of the criteria good. |
| F64 Demoförvar | 4 | | | 4 | | | Incomplete isotopes and long sections. |
| F4P1 Kemimonitering | 2 | | | 2 | | | Inadequate time or sample series; one with incomplete isotopes |
| F62 LOT | 2 | | 1 | | | 1 | Good quality. Cat. 4 incomplete for isotopes but rest of the criteria very good, |
| F91 COLLOID | 2 | | | | | 2 | Incomplete isotopes and long sections |
| KLX02 | 2 | | | | | 2 | Single samples, incomplete isotopes and 1 with a long section. |
| TBM | 2 | | | 2 | | | Incomplete isotopes and inadequate series. |
| ÄFS – svavel och multiel | 1 | | | 1 | | | Inadequate monitoring series and long section. |
| F60 2-phase flow | 1 | | | 2 | | | Incomplete isotopes and long section. |
| F61 Backfill&Plug | 1 | | | | | 1 | Incomplete isotopes |
| TUDP002 Utbyggnad | 5 | | | | | 5 | Samples taken during drilling. More samples and data were made available during the production of this report, see Appendix 4. |

Incomplete datasets are a common reason for the downgrading to a lower quality category (although the existing data could be good). A general strategy, used in many of the investigation programmes and projects that include frequent and extensive groundwater sampling, is to vary the extent of the analyses to save time and money. It is common to take a basic set of samples with a minimum of analyses (for example, excluding expensive isotopes and trace metals) as well as a limited and more exclusive set of samples for complete analyses from each sampling location. This is reflected in the categorisation and the number of samples belonging to each category over the years and in the different projects. However, there are also several other causes for an incomplete dataset, for example analytical failure, loss of a sample, a sample regarded as less important at the sampling occasion or a sample collected for a special task or check.

With respect to the different projects, the number of samples associated with them and their categories as shown in the lower panel of Figure 5-5 and explained in Table 5-4, the most relevant observations are summarised as follows:

- Most of the samples have been taken in association with the monitoring programme GWCM (around 46%) and most of them correspond to Categories 2 (32.6%) and 3 (36.9%).
- The number of samples taken during the tunnel construction was very important (together around 17% of the total) and most of them have been considered Category 3 and 3b (mainly because of the inadequate sample series and the incomplete isotopes).
- Besides the monitoring programme (GWCM), the projects F63 Prototype, Redox and F56 TRUE Block Scale have contributed with the largest amounts of high quality samples (i.e. low category number).

### 5.2.2 Data Set II: Category 5

This data set compiles those samples that do not fulfil the minimum quality criteria. When applying the categorisation process, the first and most important criteria that the samples have to satisfy before continuing the characterisation is the completeness of the major ions, without which a relevant charge imbalance cannot be calculated. Therefore, the lack of Na, Ca or Cl directly allocates the sample a Category 5 (see Chapter 4 for more details). This basic check leads to 536 samples being discarded for modelling from the beginning although the data they contain is very variable (Table 5-5) depending on the objectives of the sampling (as indicated above).

There are some additional samples that, despite having complete sets of data, they do not accomplish some of the other categorisation criteria, for example a high percent of drilling water, high charge imbalance calculated from speciation with PHREQC (> ±5%), high pH values associated with the impact from grouting, samples taken during drilling from the recycled water and not from an isolated borehole section, and samples lacking specific information as to their location. The reasons for exclusion and the number of samples in each group are indicated in Table 5-5.

Figure 5-6 shows the distribution of Category 5 samples over the years (panel above) and associated with the different projects (panel below). The highest amount of Category 5 samples correspond to 1992 (when the highest number of samples were taken over the studied period) and they represent 48% of the total groundwater samples taken that year (289 samples). They are associated mainly with the construction of the second part of the tunnel (750–3,191 m). The second highest amount of Category 5 samples correspond to 1991 but they only represent 25% of the total groundwater samples taken that year (255) as the number of good quality samples is higher. They are associated with the tunnel construction (0–750 and 750–3,191 m) and with the Redox Project. The other cases with a high percentage of Category 5 samples (with respect to the total amount of samples taken) correspond to 1996 (57% of the samples; most of them associated with F83 TRUE-1), 2006 (50%; all of them associated with F79 LTDE), 2008 and 2009 (55% and 51%, respectively and associated with GWCM).

**Table 5-5. Number of Category 5 samples included in Dataset II. Reasons for exclusion are also indicated.**

| No. sample | Reason for exclusion | Comments | |
|---|---|---|---|
| 17 | Data for all the major components except Cl | 3 samples also have a low pH values (from borehole HBH02) | Discarded since the beginning |
| 3 | Only data for cations | One of them does not have K | |
| 28 | Data for major cations (Na, K, Ca, Mg) and sulphate | One of them does not have K | |
| 23 | Only data for anions (Cl, $HCO_3^-$ and $SO_4^{2-}$) | 3 of these samples have values for Ca | |
| 8 | Only data for anions (Cl, $HCO_3^-$, $SO_4^{2-}$) and isotopes | 1 with $\delta^{18}O$, 1 with $\delta^{18}O$ and $\delta^2H$ 6 with $\delta^{18}O$, $\delta^2H$ and $^3H$ | |
| 17 | Only data for Cl | One of them with a pH value of 8.74 | |
| 1 | Only data for Cl and $SO_4^{2-}$ | pH value of 6.18 | |
| 174 | Only data for Cl and $HCO_3^-$ | 1 sample has value for Ca. Another sample has a pH value of 11.3 | |
| 135 | Only data for Cl, $HCO_3^-$, $\delta^{18}O$ and $\delta^2H$ | 79 have $^3H$ values. Two samples with high pH values (11.4 and 10.7) | |
| 3 | Only data for $HCO_3^-$ | 2 of the samples have values for $\delta^{18}O$ and $\delta^2H$.<br>1 sample with pH=10.1 | |
| 1 | Only data for $SO_4^{2-}$, $\delta^{18}O$, $\delta^2H$ and $^3H$ | | |
| 11 | Only data for Cl and S(-II) | | |
| 36 | Only data for S(-II) | | |
| 2 | Only data for Fe | | |
| 8 | Only isotopic information | 1 sample with $\delta^{18}O$, 1 sample with $\delta^{18}O$ and $\delta^2H$, and 6 with $\delta^{18}O$, $\delta^2H$ and $^3H$ | |
| 67 | No analytical data at all | | |
| 60 | High charge imbalance (> ± 5%) | All of them with complete major ions; one of them has a low pH: 6.2 | |
| 19 | Drilling water between 5 and 10% | Charge imbalance > ±5% | |
| 17 | Samples with drilling water > 10% | Charge imbalance < ±5% except for one without Cl, $SO_4^{2-}$and Na data. There is one sample with a pH=11.3 | |
| 28 | Sampling during drilling from the recycled water at the surface (Äspö extension project) | 3 samples with high pH values (between 9.97 and 10) and clearly affected by grouting | |
| 10 | Samples with pH higher than 8.7 | If there are reasons to believe that it is due to impact from grouting | |
| 3 | Lack of information or suspicious data | | |
| 674 | Total number of samples in Dataset II. | | |

The monitoring programme (GWCM) shows the highest number of Category 5 samples; however, as it is also the project with the highest number of samples taken over the studied period, these Category 5 samples only represent 18% of that total (888 samples). In a similar way, although represented by a smaller number of samples, the 750–3,191 m and Redox projects show the next highest number of Category 5 samples and, for the same reasons, they only represent 25% of the total number of samples taken.

At the other extreme are the samples taken in the Äspö extension Project, where the Category 5 samples in this case represent the 85% of the total amount of samples taken. This is a natural result of testing the relevance of sampling and analysing the recycled water during drilling, i.e. water coming out from the present borehole length while drilling and not from an isolated borehole section.

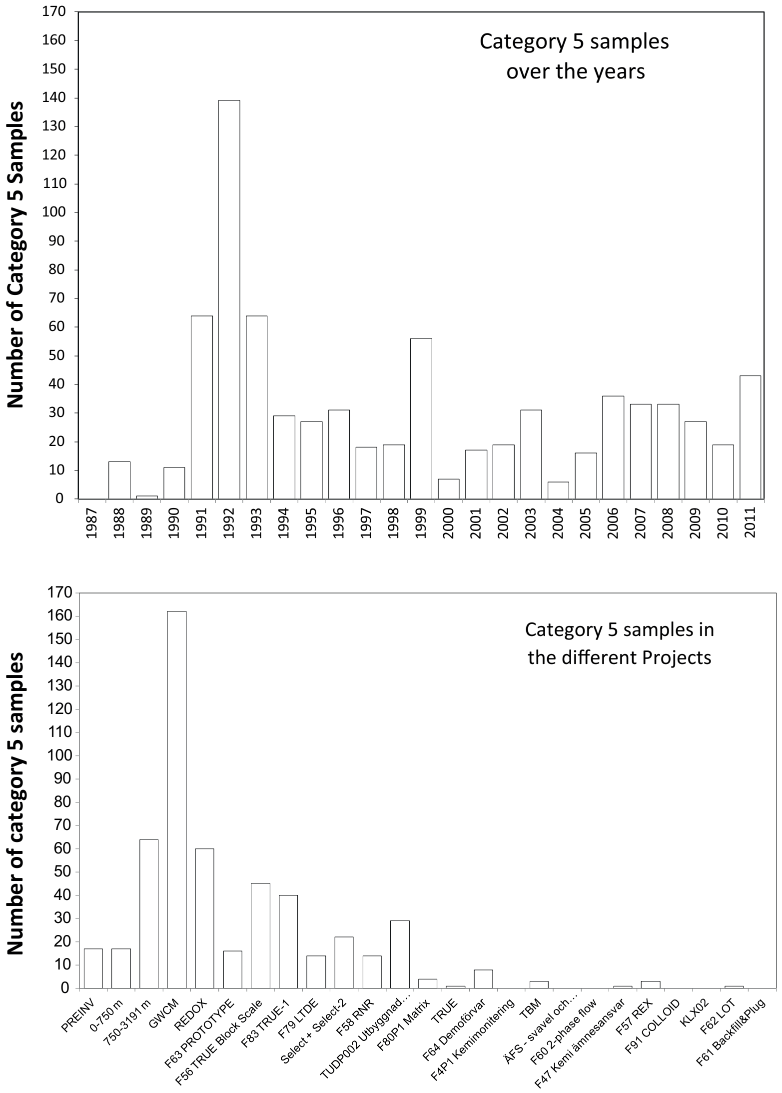

***Figure 5-6.*** *Number of samples allocated Category 5 for each year (above) and project (below) during the time period 1987 to 2011.*

## 5.3 Consistency checks

Apart from the quality analyses performed to categorise the Äspö dataset, several additional consistency checks were also made. Different calculated conductivities are compared first and then the measured conductivities are checked against the calculated ones. Something similar is done with the charge imbalance, comparing the values calculated by Sicada directly from the analytical values, with the values calculated by PHREEQC after the speciation calculation. Another check consists of the comparison between the results obtained when two different analytical techniques have been used for the same parameter (iron, uranium and sulphate cases shown below) and finally, the correlation between chloride and bromide is analysed.

### 5.3.1 Electrical conductivity and charge imbalance

Several methods have been reported for calculating the conductivity of a natural water sample from its chemical composition (see, for example, the review in Visconti et al. 2010). However, chemical speciation affects the electrical conductivity of electrolyte solutions (electrical conductivity is sensitive to the presence of aqueous complexes) and conductivity calculations need to consider the speciated concentrations instead of the analytical concentrations. Thus, a geochemical speciation model is required to perform accurate conductivity calculations (Visconti et al. 2010, McCleskey et al. 2012). Two recent methods coupled to speciation calculations have been used here to obtain theoretical conductivity values: 1) the approach by Appelo (2010) which is implemented in the PHREEQC code[2], and 2) the approach by McCleskey et al. (2012), which has been incorporated in the last version of the WATEQ4F code[3].

The conductivity values at 25 ºC obtained by both methods are shown in Figure 5-7 a and the results are completely equivalent for the range of values found at Äspö (note it will not be the same for higher salinity waters). Only 4.6% of the samples show a difference greater than 1% (430 µS/cm) between the two calculated values. This theoretical value for the conductivity could be very useful, mainly in the cases where there are not conductivity measurements (220 samples in Data Set I, around 14% of the total). If the calculated conductivity (values obtained with PHREEQC) is compared with the measured one (Figure 5-7 b) the correlation between the values is still quite good ($r^2$=0.979) although about 10.6% of the samples (145 out of 1,365 with measured values) fall outside the accepted ±5%. The supporting correlation, not shown here, is the one between these calculated values and the chloride content. It is very good ($r^2$=0.996) supporting the fact that chloride is the main ion contributing to the electrical conductivity.

Figure 5-8 shows the comparison of the Charge Imbalance calculated by Sicada just based on the analytical data, with the values obtained by PHREEQC once the speciation calculations have been done. The equivalence between them is very good ($r^2$=0.99).

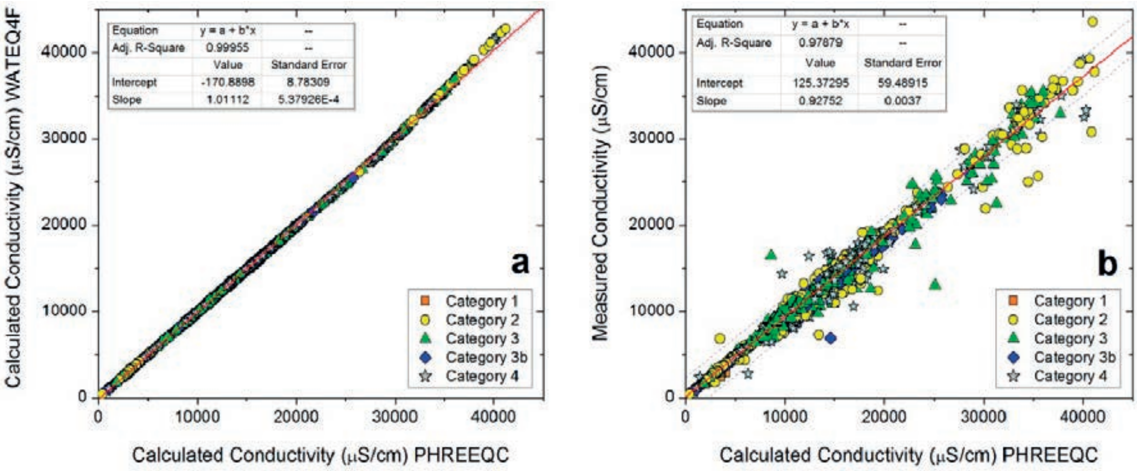

***Figure 5-7.*** *Measured and calculated electrical conductivities. (a) Comparison between the conductivity values calculated by two different approaches, one implemented in PHREEQC and the other implemented in WATEQ4F (see text for details). (b) Comparison between the measured (field and laboratory) and the calculated electrical conductivity.*

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[2] Appelo´s approach is based on the ionic molar conductivity values for the species that contribute to the electrical conductivity. It calculates the conductivity of a solution from the speciated concentrations, the activity coefficient and the diffusion coefficient of all charged species. The method has been implemented in the PHREEQC code, version 2.17.0 (from February 25, 2010) and the diffusion coefficients needed for calculations are included in the PHREEQC.dat database distributed with the code. The method takes into account the influence of temperature and provides reliable values for solutions between 10 and 60,000 µS/cm.

[3] McCleskey et al´s approach uses the ionic molal conductivities and speciated ion concentrations to calculate the conductivity values. The ionic molal conductivities of main cations and anions, some trace metals and ion pairs were obtained experimentally and the method has been incorporated to the last version of the WATEQ4F code (version 3.0 from March 10, 2011) available at http://wwwbrr.cr.usgs.gov/projects/GWC_chemtherm/software.htm.

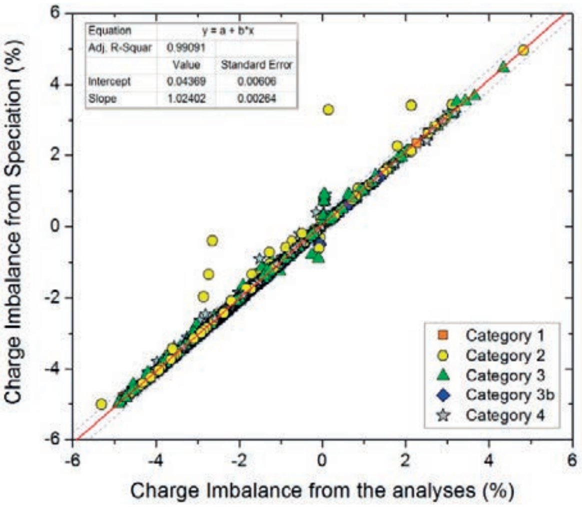

***Figure 5-8.*** *Comparison between the charge imbalance calculated directly from the analytical data and the values obtained after speciation calculations performed with PHREEQC.*

### 5.3.2 Effects of the analytical techniques

The consistency of the data can also be checked by comparing the contents of a specific element obtained using different analytical techniques. For the Äspö dataset this comparison was done in the cases of total iron, sulphate and uranium (elemental and U-238 activity).

The iron concentrations determined by ICP-AES and by a spectrophotometric method (Ferrozine) are compared in Figure 5-9a. In general, the agreement is very good between the two methods, as expressed by the r-square value (0.96). However, there are several samples with slightly different values for the two techniques. The likely explanation for the cases in which the ICP value is higher (especially at high iron concentrations), is the presence of iron bounded to a colloidal phase: the ICP method includes colloidal iron while the spectrophotometric method excludes or only partly includes colloid species. Only a few ICP values are smaller and most probably reflect the analytical error.

Both the $U^{238}$ activity and the uranium concentration have been determined in a limited amount of samples (151 and 249, respectively, and not always both in the same sample). The uranium concentrations obtained by the two methods are compared in Figure 5-9b. Generally, the agreement is very good (r-square=0.83). One Cat. 4 sample shows the largest deviation but the other diverging values are regarded as acceptable considering the low concentrations.

Sulphate by ion chromatography and sulphate calculated from total sulphur by ICP are compared in Figure 5-10a, and most samples show a satisfactory agreement. The differences increase above the sulphate content of 300 mg/L. The ICP analyses of sulphur may be affected by sulphide in the samples since sulphur increases disproportionately at high sulphide concentrations due to hydrogen sulphide gas entering the plasma. However, this is probably not the main reason for the discrepancies observed in this case.

In order to check the possible effects of using one value for sulphate or the other, an analysis was performed with PHREEQC to calculate the charge imbalance, the electrical conductivity and the TDS of the samples when using one of the values or the other. The results are shown in Figure 5-10 b, c and d. The results for the calculated conductivity and TDS show an almost perfect correlation between the values calculated with the two sulphate values, indicating that there is not much effect on the final values irrespective of the sulphate value used to obtain them. The charge balance (Figure 5-10 d) seems to be slightly more affected but, although there are several samples outside the accepted range of ±5%, the correlation between the two calculated values is 0.968. Therefore, irrespective of the sulphate value chosen for the samples, it does not make any difference in the final result in terms of charge balance or salinity of the sample.

Knowing that both values can be considered equivalent in most of the cases, the value used for each sample correspond to the sulphate calculated from total sulphur by ICP. However if it was not analysed, the value included in the final sulphate column is the sulphate obtained by ion chromatography.

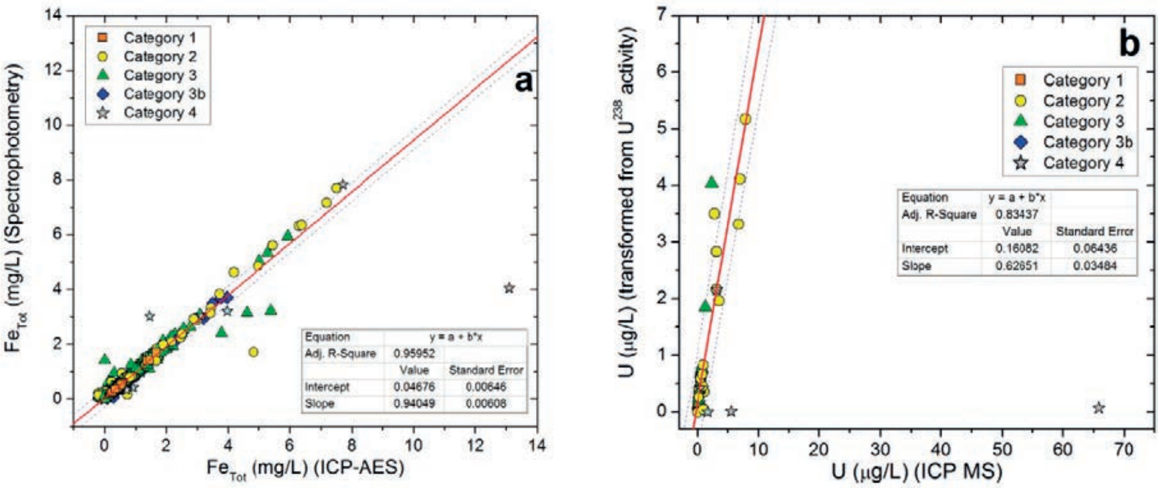

***Figure 5-9.*** *Consistency check based on the different analytical techniques used for iron (a) and for uranium (b). The uranium concentration can be calculated from the U$^{238}$ values and compared to the uranium concentration obtained by ICP MS using the relation 1 ppm U=12.4 Bq/kg $^{238}$U.*

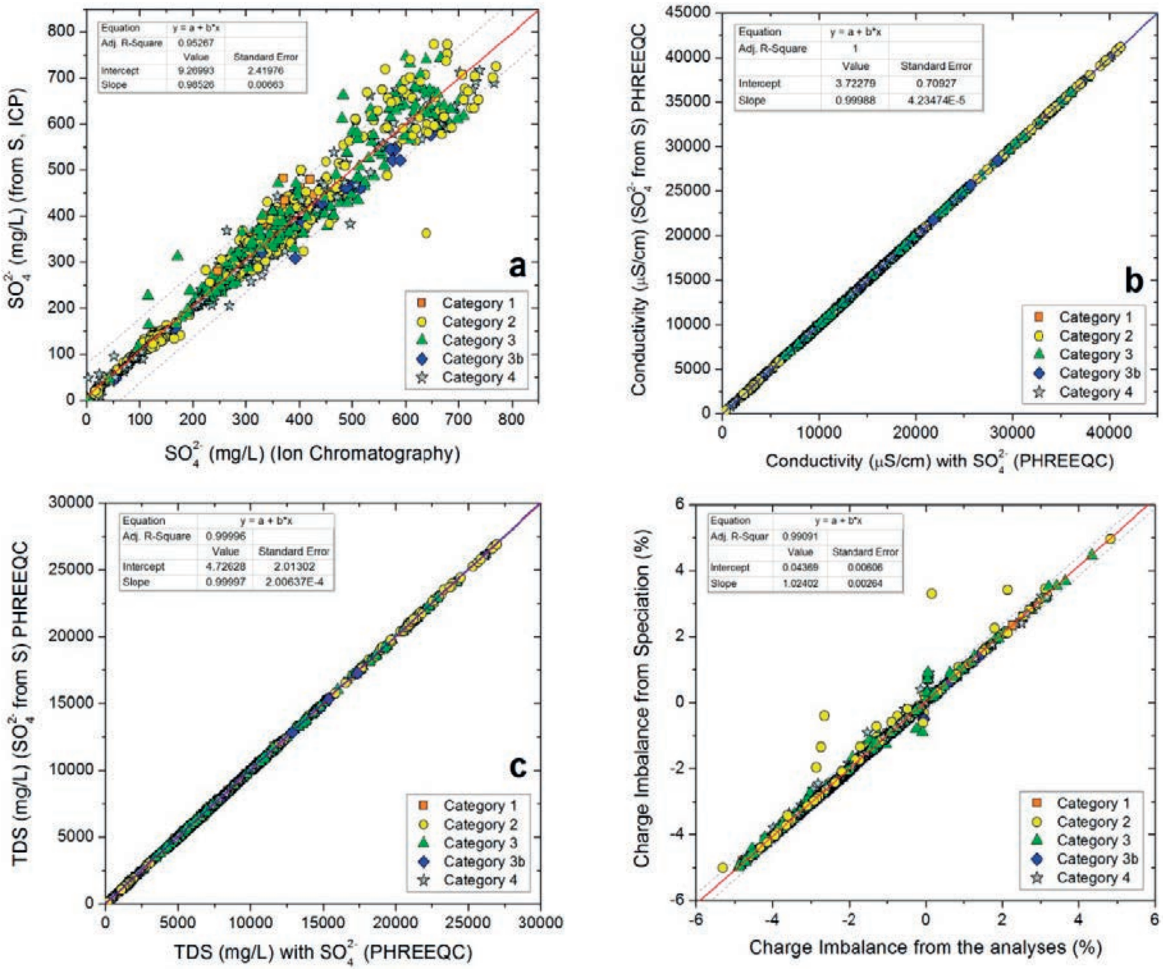

***Figure 5-10.*** *Influence of the analytical value used for sulphate. (a) sulphate content; (b, c and d) conductivity, TDS and charge imbalance calculated with PHREEQC for the two cases.*

### 5.3.3 Bromide and chloride

Selected bromide values (by IC) are plotted versus the corresponding chloride concentrations in Figure 5-11a as a rough consistency check. The corresponding points for the end member waters used in the previous site investigations (present Baltic, Littorina, glacial, altered meteoric and saline waters) are given for comparison.

Although the correlation line is quite good for the complete set of data ($r^2$=0.95), looking at the position of the end members it is quite clear that the data points form two different trends (mixing lines) and most points do not differ too much from these trend lines. The two trends correspond to marine (align with Baltic and Littorina) and non-marine origin (align with the Saline end member of Äspö), respectively. Marine waters should have a bromide/chloride ratio of approximately 0.0035 whereas ratios around 0.01 are more typical of water/rock interaction.

Additionally, as demonstrated, many of the IC analyses of bromide conducted during 2004 deviates from both possible expected trends indicating systematically erroneous and too high bromide concentrations (Figures 5-11a and b).

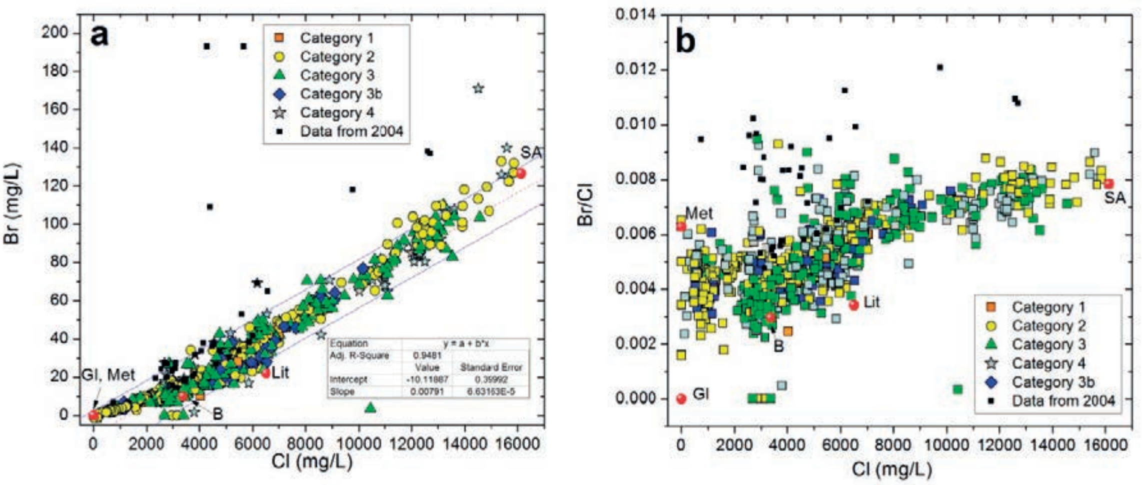

***Figure 5-11.*** *Bromide and chloride concentrations in the samples from the Äspö Data Set I. a) Bromide concentrations plotted versus chloride; and b) Br/Cl ratios versus chloride concentrations. The end member location in both plots (present Baltic, Littorina, glacial, altered meteoric and saline waters) is given for comparison (B, Lit, Gl, Met and SA).*

# 6 Object types and assessed quality categories

This chapter describes in detail the results obtained for the whole set of Äspö data (which are all included in the excel file ÄspöDataReport.xls), presenting the sampled boreholes and weirs, the samples taken from them and a summary of the information about the type of samples and their quality.

It has been organised by object types, that is, different types of boreholes as well as other sampled objects (weirs). The object types considered here are: 1) boreholes from the ground surface, 2) probing boreholes during tunnel excavation, 3) other boreholes drilled during the construction phase (involved in the principal studies/investigations), 4) project boreholes (drilled during the operational phase), and finally 5) weirs. For each group, a short description of the objects in general is presented first and then a detailed relation of the amount of boreholes included in the group, the sections and samples taken in them, their categories, and finally one or several tables including all this information systematically.

## 6.1 Boreholes from the ground surface

### 6.1.1 Description

The percussion and cored boreholes from the surface inside the study area (cf. Figure 3-1) were drilled during the pre-investigation phase (1986 to 1990) except for the three percussion boreholes on Bockholmen (HBH01, HBH02 and HBH05) that were drilled for the Redox Project during the construction phase), see Section 2.1. The boreholes included in this group are listed in Table 6-1.

**Table 6-1. Cored and percussion boreholes from ground surface in Äspö and Bockholmen.**

| Äspö | | Bockholmen | |
|---|---|---|---|
| **Percussion boreholes** | **Cored boreholes** | **Percussion boreholes** | **Cored boreholes** |
| HAS02<br>HAS03<br>HAS05<br>HAS06<br>HAS07<br>HAS09<br>HAS13<br>HAS14<br>HAS18<br>HAS19 | KAS02<br>KAS03<br>KAS04<br>KAS05<br>KAS06<br>KAS07<br>KAS08<br>KAS09<br>KAS11<br>KAS12<br>KAS13<br>KAS14 | HBH01 Redox<br>HBH02 Redox<br>HBH05 Redox | KBH02<br>KBH02T<br>KBH02 was an almost horizontal borehole drilled parallel to the planned access tunnel direction. It was later on intercepted by the tunnel construction, and consequently given the new name of KBH02T. |

Core drilling was conducted using a new technique known as telescopic-type drilling. This implies that the uppermost 100 m of the borehole is reamed up to 155 mm diameter while the rest of the borehole is 56 mm or 76 mm (Almén and Zellman 1991). This allowed contemporary air-lift pumping to be conducted in the wide part of the borehole during the continued drilling which has the important advantage of reducing the intrusion/contamination of flushing water and drilling debris into the surrounding formation groundwater. The flushing water was taken from a percussion borehole in the same rock formation and coloured by Uranine (1.0 mg/L). Groundwater sampling in the cored boreholes has been conducted using four different methods (see Table 2-2):

1) **Sampling during drilling.** Samples collected during drilling were contaminated by a large contribution of flushing water and were generally found to belong to Category 5: see 4.2.1. Otherwise they would have been very important as first strike samples prior to continued drilling to greater depths and later by the general impact of the borehole presence itself and possibly even more so by borehole activities such as downhole hydraulic testing and geophysical measurements.

2) **Sampling during pumping tests.** This method consists of pumping at high flow rates (several litres per minute) through an aluminium pipe string. This may have had some impact on the sample quality.

3) **Sampling for complete hydrochemical characterisation (CCC).** This is the most advanced sampling method and it was performed in selected cored boreholes using the mobile chemistry unit which comprises an integrated system for: a) isolation of a borehole section and pumping of groundwater from the section; b) sampling of pumped groundwater as well as sampling *in situ* in the borehole section at maintained pressure; and b) on-line long-term measurements (weeks or months) of pH, Eh, water temperature, EC and dissolved oxygen (Almén and Stenberg 2005, Smellie and Laaksoharju 1992). In contrast to the procedure followed during the PLU, the CCC sampling conducted at Äspö was often late in the investigation sequence. This, and the probability of excess hydraulic pumping prior to sampling (Smellie and Laaksoharju 1992), may have influenced the results.

4) **Long term monitoring sampling.** Groundwater sampling to monitor the hydrogeochemical conditions and identify changes has continued in selected borehole sections (circulation sections) using stationary packer equipment until drawdown or deterioration of the downhole equipment made it impossible. Generally, five section volumes of groundwater were pumped out before sampling. It has been proved subsequently during the monitoring programme in Forsmark in 2009 that this is most often insufficient in order to obtain representative samples containing groundwater from the bedrock formation (Nilsson et al. 2010, Tullborg et al. 2010a, b). The volume that should be discharged was found to be specific for each borehole and dependent on the number and location of the water yielding fractures along the borehole section and their hydraulic transmissivity as well as the section length (see Section 2.4.4). Insufficient discharge before sampling was found to be critical not only for the sulphide concentrations, but also TOC/DOC and trace metals also may have been affected.

Most of the percussion boreholes were drilled early in the investigations in 1987 to get a rough idea of the hydraulic character and the hydrogeochemical situation in the area. Borehole lengths were normally between 100 to 200 m and the dip angles were between 55° and 90° from the horizontal axis. The most common diameter was 115 mm but some of the boreholes were 165 mm. Groundwater sampling was conducted immediately after the boreholes were drilled and the samples are, therefore, expected to be reasonably representative of the situation in the undisturbed rock (Almén and Zellman 1991). Light portable pump and single packer equipment was used for the sampling in this first batch of percussion boreholes (Almén and Zellman 1991). The packer was placed between 20 and 80 m down in the borehole depending on the location of the water conducting fractures. Two samples were collected, the first one half an hour after the pump was started and the second one 24 h later when between 1 and 8 cubic metres of water had been pumped out of the borehole section. From the subsequently drilled boreholes sampling was performed only in HAS13 (CCC), however, samples have been collected later on (2005) from some of the other boreholes.

### 6.1.2 Results from quality assessment

There are 27 boreholes included in this "object type": 3 percussion boreholes and 1 cored borehole in Bockholmen, and 10 percussion boreholes and 13 cored boreholes at Äspö (see Table 6-1) and a total of 446 groundwater samples were taken from them, 380 from Äspö (mainly during the pre-investigation research phase, but also during the monitoring programme and within the framework of project F47 Kemi ämnesansvar) and 66 from Bockholmen (taken during the Redox Project, as part of the GWCM and during the tunnel construction, 750–3,191 m). All data indicate adequate time or sample series with more than 4 samples. The number of samples included in Data Set I is 375 from which 138 are considered representative of the Initial Conditions. Due to the long sections and the incomplete data for isotopes, most of these samples have been evaluated as Category 4 samples. There is only one Category 1 sample, 42 Category 2, 69 Category 3, 34 Category 3b and 229 Category 4. Additionally, there are 71 Category 5 samples associated with some of these boreholes which have incomplete major ions or, if complete, the charge imbalance is high (Table 6-2).

**Table 6-2. Boreholes, sections (including the elevation, m.a.s.l., at the middle of the section) and samples corresponding to the boreholes included in this object type (boreholes from the ground surface). The column with comments indicate some specific information about the samples. Some abbreviations are used in this column in order to shorten the text: Cat for Category, DSI and DSII for Data Sets I and II, CI for charge imbalance, init. cond. for initial conditions and series for sample or time series.**

| Borehole ID, section and vertical elevation (mid sec) | Tot no. | Number of samples in each category. | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **Äspö (percussion boreholes)** | | | | | | | | |
| HAS02 (–56.12) 44–93 | 2 | | | | | 2 | | Short time series (2 days) and long sections (Cat. 4). All of them correspond to the Pre-investigation project (Preinv) and they have been considered representative of the initial conditions (init. cond.). |
| HAS03 (–60.13) 48–100 | 2 | | | | | 2 | | |
| HAS05 (–56.26) 45–100 | 2 | | | | | 2 | | |
| HAS06 (–65.03) 40–100 | 2 | | | | | 2 | | |
| HAS07 (–75.02) 71–100 | 2 | | | | | 2 | | |
| HAS09 (–9.48) 0–40 | 1 | | | | | 1 | | No series and long section (Cat 4). Sampled in 2005 associated with F47 Kemi ämnesansvar. |
| HAS13 (–64.88) 51–100 | 4 | | | 1 | | 3 | | Better time series (4 days) but worse in isotopes. Preinv samples considered Init. cond. |
| HAS14 (–48.27) 0–100 | 7 | | | | | | 7 | All Cat. 5: mainly incomplete major ions. Sampled in 2005 associated with F47 Kemi ämnesansvar. |
| HAS18 (–7.92) 0–35 | 2 | | | | | 1 | 1 | No series, long section (Cat 4) and incomplete major ions (Cat. 5). Sampled in 2005 associated with F47 Kemi ämnesansvar. |
| HAS19 (–7.89) 0–40 | 1 | | | | | 1 | | No series and long section (cat 4). Sampled in 2005 associated with F47 Kemi ämnesansvar. |
| **Äspö (cored boreholes)** | | | | | | | | |
| **KAS02** | 64 | 1 | 3 | 3 | 8 | 49 | 11 | Several sections. Eleven samples discarded and stored in Data Set II (DSII; Cat 5) because of the incomplete major ions and some high charge imbalance (between 5 and 10%). Most of the samples were taken during the Preinv. programme, but there are also some samples from the monitoring GWCM. |
| (–199.81) 202–214 | 10 | | 1 | | 6 | 2 | 1 | Good time series and short section. Incomplete isotopes data (Cat. 3b) and incomplete major ions (Cat. 4). Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All these samples are considered representative of init. cond. One Cat. 5 sample: CI > 5%. |
| (–307.69) 314–319 | 8 | | 1 | | 1 | 5 | 1 | Good time series and short section. Incomplete isotopes data (Cat. 3b) and incomplete major ions (Cat 4). Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All these samples are considered representative of init. cond. One Cat. 5 sample: incomplete major ions. |
| (–317.15) 308–344<br>(–318.15) 309–345 | 14 | | | 1 | | 12 | 1 | These two sections include the previous one. Good time series, charge balance and low% drilling water but long sections and incomplete isotopes (sometimes even incomplete major ions). 2 sampling periods for the two different sections (Preinv, 4 samples considered representative of init. cond., and GWCM from 1990 to 1992, 10 samples). One sample of Cat. 3 was selected as representative during the PLU at the end of the time series. One Cat. 5 sample: CI > 5%. |
| (–456.16) 463–468 | 0 | 1 | | | 1 | 5 | 2 | Incomplete isotopes (Cat 3b) and incomplete major ions (cat 4). The rest of the criteria are very well accomplished. Sample of Cat. 1 selected as representative during the PLU at the end of the time series. All samples considered init. cond. (Preinv). Two Cat, 5 samples: Incomplete major ions and CI > 5%. |
| (–522.95) 530–535 | 5 | | 1 | | | 2 | 2 | Cat. 4 samples due to incomplete major ions and incomplete isotopes data in one of the samples. Sample selected as representative during the PLU was at the end of the time series, here the second sample is considered Cat 2. Two Cat. 5 samples: incomplete major ions and CI > 5%. |

| Borehole ID, section and vertical elevation (mid sec) | Tot no. | Number of samples in each category. 1 | 2 | 3 | 3b | 4 | 5 | Comments |
|---|---|---|---|---|---|---|---|---|
| (–816.46) 800–854 | 13 | | | 1 | | 9 | 3 | Samples taken during the monitoring programme GWCM from 1990 to 1992. The last sample of the monitoring series has been labelled as Cat.3. The rest are considered Cat 4 due to the long section and the incomplete isotope data. Three samples discarded (Cat.5 due to incomplete major ions). |
| (–852.34) 802–924<br>(–881.22) 860–924 | 16 | | | 1 | | 14 | 1 | Good time series but long section. 2 sampling periods for the two sections (Preinv, 4 samples in 1988 and 11 in 1989, all considered representative of init. cond.). Incomplete isotopes data. Two samples were selected as representative during the PLU at the end of each time series, only the last one has been considered Cat.3 here. One Cat. 5 sample due to incomplete major ions. |
| **KAS03** | 91 | | 3 | 19 | 10 | 53 | 6 | Several sections. 85 samples in Data Set I (DSI) and 6 samples in DSII (Cat. 5) due to a high percent of drilling water (two of them) and a high charge imbalance (3 of them), and the last one has a high pH value (higher than 8.7). |
| (–121.78) 129–134 | 9 | | 1 | | 8 | | | Cat 3b because of the incomplete isotope data. The rest of the parameters are good quality. Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All the samples are considered representative of init. cond. |
| (–169.44) 107–252 | 15 | | | | | 15 | 1 | Cat 4 due to the section length, the rest of the parameters are quite good. Sampled during the monitoring programme GWCM between 1994 and 2011. One Cat. 5 sample due to its high pH. |
| (–198.73) 196–222 | 4 | | | 1 | | 2 | 1 | Cat 4 due to the section length and the incomplete isotope data. Sample of Cat. 3 selected as representative during the PLU at the end of the time series. All considered init. cond. (Preinv). One Cat. 5 sample due to high percent of drilling water (between 5 and 10%). |
| (–238.92) 248–251 | 3 | | 1 | | 2 | | | Relatively good samples except for the incomplete isotopes data in two samples (Cat 3b). Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All considered init. cond. (Preinv), |
| (–348.56) 347–373 | 4 | | | 1 | | 2 | 1 | Long section and incomplete isotopes. Sample of Cat. 3 selected as representative during the PLU at the end of the time series. All considered init. cond. (Preinv), One Cat. 5 sample due to high percent of drilling water (between 5 and 10%). |
| (–454.25) 453–480 | 4 | | | 1 | | 3 | | Long section and incomplete isotopes. Sample of Cat. 3 selected as representative during the PLU at the end of the time series. All considered init. cond.(Preinv), |
| (–566.28) 533–626 | 30 | | | 16 | | 12 | 2 | Cat 3 due to the long section. Cat 4 due to the incomplete isotopes and in some cases also incomplete major ions. Sampled during the monitoring programme GWCM between 1990 and 2011. Two Cat. 5 samples due to incomplete major ions and high charge imbalance. |
| (–602.45) 609–623 | 4 | | 1 | | | 3 | | This section is included in the previous one but waters were sampled during the Preinv. programme (1988).therefore they have been considered representative of init. cond. Cat 4 due to the incomplete isotopes and major ions and the long section. Sample of Cat. 2 selected as representative during the PLU at the end of the time series. |
| (–830.02) 690–1,002<br>(–914.04) 860–1,002 | 17 | | | | | 16 | 1 | Different section lengths, Preinv programme (3 samples in 1988 and 13 in 199 in a shorter section, init. cond). All Cat. 4 due to the length of the sections and the incomplete isotopes and major ions. Samples at the end of the time series during the Preinv. programme were selected as representative during the PLU. One Cat. 5 samples due to a high Cl. |
| **KAS04** | 31 | | 2 | 2 | 13 | 9 | 5 | Several sections. 26 samples in DSI, 5 samples in DS II (contain a high percent of drilling water) but they correspond to sections different from the ones selected for DSI. Except for one of the sections, the rest of the samples were taken during the Preinvestigation programme (init. cond.). |

| Borehole ID, section and vertical elevation (mid sec) | Tot no. | Number of samples in each category. | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| (–185.15) 226–235 | 8 | | 1 | | 7 | | | Very good quality samples except for the incomplete isotopes data (Cat. 3b). Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All samples are considered init. cond. |
| (–275.61) 334–343<br>(–295.15) 332–392 | 12 | | 1 | 1 | 6 | 4 | | Two sampling occasions with different section lengths, 7 during the Preinv. programme (1989, considered init. cond.) and 5 during the monitoring GWCM (1991–1992; the longest section). Cat 3b due to the incomplete isotopes (the rest is good quality) and Cat 4 also due to the long section. Sample of Cat. 2 selected as representative during the PLU at the end of the time series during the Preinv. programme. |
| (–376.76) 440–480 | 6 | | | 1 | | 5 | | Cat 4 due to the incomplete isotopes and the long section (one also have incomplete major ions). Sample of Cat. 2 selected as representative during the PLU at the end of the time series. All are considered representative of the init. cond. |
| **KAS05** | 15 | | | 1 | | 10 | 4 | Several sections. 11 samples in DSI and 4 samples in DSII (Cat 5 due to the high percentage of drilling water, higher than 10 except 1 higher than 5). All the samples have been taken during the monitoring GWCM programme. |
| (–319.57) 307–353<br>(–339.44) 320–380 | 7 | | | 1 | | 4 | 2 | Two sampling occasions 1990–1991 and then 1992 and 1994. Cat. 4 due to the incomplete isotope data and the very long sections. Two Cat. 5 samples. |
| (–473.86) 421–549.6<br>(–483.29) 440–549.6 | 8 | | | | | 6 | 2 | Two sampling occasions 1990–1991 and then 1992 and 1994. Cat. 4 due to the incomplete isotope data and the very long sections. Two Cat. 5 samples. |
| **KAS06** | 27 | | 1 | 4 | 3 | 19 | | Several sections. Not very good quality due to the long sections and the incomplete isotopes. |
| (–182.66) 191–249<br>(–200.04) 204–277 | 8 | | | 2 | | 6 | | Two sampling occasions with different sections, one during the Preinv. programme, 4 samples in 1989 (considered init. cond.), and the other during the monitoring GWCM programme with another 4 samples taken between 1990 and 1992. Similar qualities in both cases. Cat 3 in the Preinv group was selected as representative after the time series and because of the isotope data. |
| (–284.37) 304–377 | 4 | | | 1 | | 3 | | Cat 4 due to the long sections and the incomplete isotopes. Cat 3 in the Preinv group was selected as representative after the time series and because of the isotope data. All samples considered representative of init. cond. |
| (–331.85) 389–406 | 4 | | 1 | | 3 | | | Better categories (2 and 3b) because of a shorter section. Cat 2 was selected as representative. All samples considered representative of init. cond. |
| (–388.03) 431–500<br>(–433.25) 439–602 | 11 | | | 1 | | 10 | | Two sampling occasions with different sections, one during the Preinv. programme, 4 samples in 1989 (considered init. cond), and the other during the monitoring GWCM programme with 7 samples taken between 1990 and 1992. Similar low qualities in both cases because of the long sections, the incomplete isotopes and some incomplete major ions. |
| **KAS07** | 26 | | | 3 | | 22 | 1 | Two very long sections. 25 samples in DSI and 1 sample in DSII due to incomplete major ions. All the samples were taken during the monitoring programme GWCM between 1990 and 1994. |
| (–201.24) 191–290 | 12 | | | 3 | | 9 | | Very long section. Cat. 3 samples have reasonable good values for the rest of the criteria. Samples from Cat 4 have incomplete isotope data and 3 have incomplete major ions. |
| (–464.86) 501–604 | 14 | | | | | 13 | 1 | Very long section. All the samples are cat 4 because of the incomplete isotope data and 2 have incomplete major ions. One Cat. 5 sample due to incomplete major ions. |
| **KAS08** | 18 | | | 2 | | 10 | 6 | Two long sections. 12 samples in DSI, 6 samples in DSII (mainly due to a high percent of drilling water). All the samples were taken during the monitoring programme GWCM between 1990 and 1994. Long sections and incomplete isotope data. |
| (–135.85) 140–200 | 8 | | | | | 4 | 4 | |
| (–441.28) 503–601 | 10 | | | 2 | | 6 | 2 | |

| Borehole ID, section and vertical elevation (mid sec) | Tot no. | Number of samples in each category.<br>1 | 2 | 3 | 3b | 4 | 5 | Comments |
|---|---|---|---|---|---|---|---|---|
| **KAS09**<br>(–110.56) 116–150 | 27 | | | 23 | | 4 | | All the samples taken during the monitoring programme GWCM between 1990 and 2011. Good quality and quite complete data (including isotopes) but still very long section. |
| **KAS11** | 6 | | | | | 6 | | Two sections. All the samples were taken during the monitoring programme GWCM in 1991. Incomplete isotope data and long sections. |
| (–51.24) 47–64 | | | | | 3 | | | 3 good samples but incomplete isotopes. Drilling water content unknown. |
| (–163.73) 153–183 | | | | | | 3 | | Not very good samples due to the long sections (apart from the incomplete isotopes). Drilling water content unknown. |
| **KAS12** | 12 | | | 3 | | 9 | | Two sections. All the samples were taken during the monitoring programme GWCM between 1991 and 1993. Incomplete isotope data and long series (Cat. 4). |
| (–231.63) 234–277 | 6 | | | 3 | | 3 | | 3 good samples except for the long section (Cat 3) but taken at the end of the monitoring series. The other three have also incomplete isotopes (Cat 4). Drilling water content unknown in all of them. |
| (–275.57) 278–329 | 6 | | | | | 6 | | Long section and incomplete isotopes and major ions data. |
| **KAS13** | 11 | | | 1 | | 6 | 4 | Two sections. 7 samples in DSI and 4 samples in DSII (due to a high charge imbalance). All the samples were taken during the monitoring programme GWCM between 1991 and 1992. Incomplete isotopes data and long series (Cat.4).<br>Long sections and incomplete isotopes except in the Cat. 3 sample that could be considered reasonably good after the monitoring series. |
| (–146.29) 151–190 | 5 | | | | | 3 | 2 | |
| (–176.87) 191–220 | 6 | | | 1 | | 3 | 2 | |
| **KAS14** | 10 | | | 2 | | 8 | | Two sections. All the samples were taken during the monitoring programme GWCM between 1991 and 1992. Incomplete isotope data and long series (Cat. 4). |
| (–112.2) 131–138 | 5 | | | 1 | | 4 | | Reasonably good samples except for the incomplete isotopes but adequate length of the section and monitoring give Cat. 3 to one sample. |
| (–134.82) 147–175 | 5 | | | 1 | | 4 | | Similar in quality to the previous section but the section is very long (Cat. 4), only one sample gets Cat 3 after the monitoring series. |
| **KAS16** | 6 | | | | | | 6 | Several sections. All the samples are in Data Set II and they were taken during the monitoring programme GWCM between 1991 and 1992. Incomplete major ions. |
| **Bockholmen (percussion boreholes)** | | | | | | | | |
| **HBH01** | 30 | | 18 | 4 | | 3 | 5 | Several sections. 25 samples in DSI and 5 in DSII (due to incomplete major ions and to high charge imbalance). All the samples (except the last one taken in 1995 during the monitoring programme GWCM, one of the cat. 5) were taken during the Redox Project between 1991 and 1994. |
| (–6.43) 13–13<br>(–19.50) 28–28<br>(–38.24) 49–49 | 4 | | | | | 3 | 1 | 4 different sections with single samples. Incomplete isotope data and incomplete major ions (Cat. 4 and Cat. 5). |
| (–30.85) 31–50.6 | 26 | | 18 | 4 | | | 4 | Good quality samples. Only 6 with incomplete isotope data (Cat 3). |
| **HBH02**<br>(–7.32) 0–32.4<br>(–15.27) 21–32.4 | 12 | | 10 | 1 | | 1 | 13 | Two sections. 12 samples in Data Set I and 13 samples in Data Set II (Cat., 5 due to the lack of Cl). Except the latest sample (taken in 1995), all the samples were taken during the Redox Project between 1991 and 1993.Good quality samples. Only the first one is Cat.4 due to the section length and the inadequate time or sample series. |
| **HBH05**<br>(–8.67) 11–22 | 6 | | 5 | | | | 1 | One sample discarded (Cat. 5) due to incomplete major ions (no Cl). Three samples were taken during tunnel construction (70–3,191) between 1992 and 1993 and the other 2 during the Redox project during 1993.Good quality samples. |
| **Bockholmen (cored boreholes)** | | | | | | | | |
| **KBH02T**<br>(–167.97) 0–373<br>(–194.06) 240–373 | 5 | | | | | 4 | 1 | Two sections. 4 samples in DSI and 1 sample in DSII (incomplete major ions). Samples were taken while the tunnel construction (70–3,191) between 1991 and 1993. Cat 4 due to the long section. |

## 6.2 Probing boreholes (Sonderingshål)

### 6.2.1 Description

Approximately 20 m long probing boreholes (Ø 57 mm) were percussion drilled every 16th metres on each side of the working face (front) in the excavation tunnel (Almén et al. 1994, Almén and Stenberg 2005). The probing holes were directed 20° out from the tunnel wall and parallel to the bottom of the tunnel, i.e. pointing slightly downwards (Figure 6-1). The drilling was performed at a distance of about 4 m from the tunnel front at the moment of the drilling. Immediately after drilling, a single packer (6 m) with valve arrangements was installed to isolate the borehole. Groundwater sampling was performed as a routine procedure from the boreholes with the highest flow in each borehole pair (left or right side) in conjunction with pressure build-up tests.

The results from this first sampling occasion may be considered as relatively undisturbed from the tunnel construction or the presence of the tunnel and is therefore important for the interpretation of the initial conditions. Unfortunately, the first sample from probing boreholes included a reduced set of analyses excluding isotopes in most of the cases which restricts somewhat the interpretation. These samples have, generally, been categorised as Category 3b.

### 6.2.2 Results from quality assessment

The total number of drilled probing boreholes is 128 and the number of samples taken is 575. However, 189 of these samples have been categorised as Category 5 and, therefore, they are included in Data Set II. 103 of them correspond to 34 boreholes whose samples are all Category 5 and there are no samples from these boreholes in Data Set I. They are listed in Table 6-3 together with the number of samples taken in each borehole. The other 86 samples of Category 5 correspond to boreholes that have other good quality samples stored in Data Set I; these samples will be considered in the corresponding borehole description (Tables 6-5 to 6-7).

The list of the 94 boreholes included in Data Set I is shown in Table 6-4. These boreholes (as it will be for the rest of the boreholes in the HRL tunnel) have been separated into three groups depending on the number of samples that have been taken over the time. The first group corresponds to the single sample cases and are included in Table 6-5. The second group corresponds to the boreholes with between 2 to 4 samples, and are listed in Table 6-6. And the third group corresponds to the boreholes with more than 4 samples described in detail in Table 6-7.

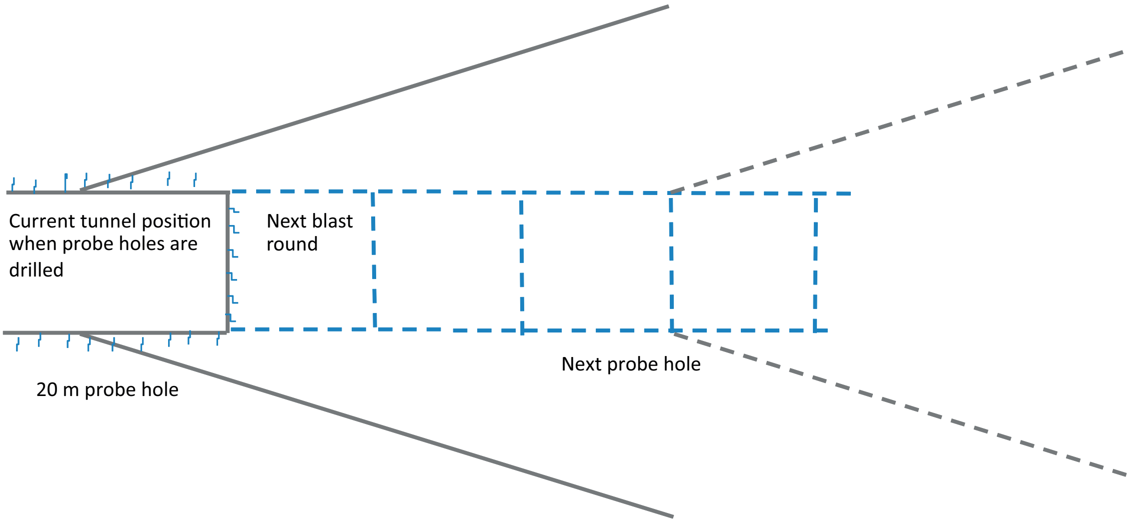

*Figure 6-1. Progress of tunnel construction viewed from the top with probing boreholes drilled at the front and ahead of four blasting rounds (modified from Almén and Stenberg 2005).*

**Table 6-3. Probing boreholes only included in DataSet II (all samples have been categorised as Category 5).**

| ID code | No. samples | ID code | No. samples | ID code | No. samples |
|---|---|---|---|---|---|
| SA0709B | 1 | SA1247B | 13 | SA2751A | 1 |
| SA0722A | 1 | SA1328A | 1 | SA2897A | 1 |
| SA0776B | 2 | SA1377F | 1 | SA2912A | 1 |
| SA0867B | 1 | SA1564B | 1 | SA3108A | 1 |
| SA0993B | 1 | SA1581A | 1 | SM0024B | 1 |
| SA0293F | 1 | SA1643B | 1 | SM00231 | 1 |
| SA1111A | 1 | SA1713A | 1 | SM0032A | 1 |
| SA1128B | 1 | SA2090B | 1 | SM00351 | 1 |
| SA1195A | 14 | SA2142B | 1 | SM00401 | 1 |
| SA1195B | 16 | SA2222B | 1 | SM00452 | 2 |
| SA1210B | 15 | SA2565B | 1 | | |
| SA1229B | 14 | SA2734A | 1 | | |

**Table 6-4. Probing boreholes included in Data Set I. They are described in detail in Tables 6-5 to 6-7.**

| | | | | | | |
|---|---|---|---|---|---|---|
| SA0158A | SA0344A | SA0976A | SA1420A | SA1997A | SA2583A | SA2834B |
| SA0205A | SA0361B | SA0976B | SA1614B | SA2025A | SA2600A | SA2880A |
| SA0221A | SA0377A | SA0992A | SA1680A | SA2074A | SA2600B | SA3045A |
| SA0237B | SA0435A | SA1009A | SA1163B | SA2074B | SA2634B | SM0024B |
| SA0267F | SA0452A | SA1009B | SA1195B | SA2109B | SA2649A | SM0032A |
| SA0271B | SA0468A | SA1062B | SA1199F | SA2142B | SA2663B | SM00352 |
| SA0285F | SA0722B | SA1077A | SA1680B | SA2175B | SA2664A | SM00451 |
| SA0289A | SA0813A | SA1094A | SA1693F | SA2192B | SA2681B | SM00452 |
| SA0289B | SA0813B | SA1145B | SA1696B | SA2240B | SA2681A | SM00456 |
| SA0293F | SA0831A | SA1210A | SA1730A | SA2273A | SA2703A | SM00457 |
| SA0311A | SA0831B | SA1229A | SA1742A | SA2273B | SA2718A | |
| SA0311B | SA0850B | SA1298F | SA1828B | SA2289B | SA2768A | |
| SA0327A | SA0923A | SA1327B | SA1844B | SA2322A | SA2768B | |
| SA0327B | SA0958B | SA1342B | SA1861A | SA2355B | SA2783A | |

There are 47 probing boreholes that have only one sample in Data Set I. 42 of them were sampled only once and 6 have another sample in Data Set II. From the total of 47 samples, 33 of them have been categorised as Category 3b with very good grades for the percentage of drilling water (1 or 2), the charge balance (1), the section length (2), and the ions (2). Variable grades with respect to the isotopes (13 samples have a 2, 14 a 3 and 21 a 4), but most of them have a 4 in the criteria related to sample or time series. Then there are another 14 samples that have been included in Category 4 and not in 3b because of the section lengths (very large).

Samples in this group were taken between 1990 and 1994 and most of them associated with the project 750–3,191 (the construction of the second part of the tunnel), but also to 0–750 m and KLX02. There is also one sample that was taken in 1998 during the monitoring programme (GWCM). Together with the surface boreholes, the probing boreholes contain the highest number of samples considered representative of the initial conditions in the system. There are 40 samples in this group of single sampled boreholes.

Apart from these samples included in DataSet I, there are 6 samples taken in some of these boreholes that belong to Category 5 (indicated in Table 6-5) mainly due to the incomplete major ions (in one case the major ions are complete but the charge imbalance is higher than 5).

**Table 6-5. List of probing boreholes with only one sample taken (or left in Data Set I). The table includes information about the ID number of the sample in Data Set I, the ID code of the borehole, the sample number, the section and its central elevation, the sampling data, the project which the sampling was associated with, the defined category and the indication of whether the sample is representative or not of the initial conditions.**

| ID DS I | ID code | Sample no. | Secup | Seclow | Elev. (m.a.s.l.) | Start date | Project | Category | Init. cond. |
|---|---|---|---|---|---|---|---|---|---|
| 836 | SA0221A | 13141 | 5.90 | 19.90 | –31.60 | 1990/12/06 | 0–750 m | 3b | y |
| 842 | SA0267F | 13143 | 0.00 | 20.70 | –37.24 | 1990/12/19 | 0–750 m | 4 | y |
| 845 | SA0285F | 13145 | 0.00 | 19.60 | –39.35 | 1991/01/10 | 0–750 m | 3b | y |
| 846 | SA0289A | 13147 | 6.00 | 19.90 | –41.13 | 1991/01/17 | 0–750 m | 3b | y |
| 875 | SA0377A | 276 | 6.00 | 20.00 | –53.46 | 1991/05/30 | 0–750 m | 3b | y |
| 890 | SA0722B | 280 | 0.00 | 20.40 | –101.62 | 1991/06/06 | 0–750 m | 4 | y |
| 914 | SA0867A | 13285 | 5.70 | 19.50 | –119.82 | 1991/11/13 | 750–3,191 m | 3b | y |
| 923 | SA0976A | 148 | 1.00 | 20.00 | –134.46 | 1991/11/19 | 750–3,191 m | 3b | y |
| 926 | SA0992A | 147 | 0.20 | 16.50 | –136.36 | 1991/11/18 | 750–3,191 m | 3b | y |
| 927 | SA1009A | 2655 | 6.00 | 19.50 | –139.72 | 1998/10/01 | GWCM | 4 | |
| 947 | SA1077A | 13309 | 6.00 | 20.40 | –149.29 | 1992/04/23 | 750–3,191 m | 3b 5 | y |
| 948 | SA1094A | 13310 | 4.50 | 20.00 | –151.55 | 1992/04/23 | 750–3,191 m | 3b 5 | y |
| 949 | SA1111B | 13311 | 6.00 | 19.00 | –155.04 | 1992/04/23 | 750–3,191 m | 3b | y |
| 950 | SA1145B | 139 | 6.00 | 19.90 | –158.56 | 1992/01/20 | 750–3,191 m | 3b | y |
| 951 | SA1163B | 89 | 6.00 | 20.00 | –161.53 | 1992/05/18 | 750–3,191 m | 3b | y |
| 952 | SA1199F | 136 | 0.00 | 40.00 | –167.55 | 1992/02/04 | 750–3,191 m | 4 | y |
| 975 | SA1298F | 13312 | 0.00 | 39.50 | –178.62 | 1992/05/04 | 750–3,191 m | 4 | y |
| 976 | SA1327B | 2023 | 6.00 | 20.30 | –184.06 | 1992/10/15 | 750–3,191 m | 3b | y |
| 977 | SA1342B | 84 | 0.00 | 20.30 | –186.54 | 1992/06/16 | 750–3,191 m | 4 | y |
| 1007 | SA1680A | 77 | 0.00 | 16.00 | –229.24 | 1992/10/13 | 750–3,191 m | 3b | y |
| 1008 | SA1680B | 2066 | 6.00 | 20.00 | –230.30 | 1993/02/03 | 750–3,191 m | 3 5 | |
| 1009 | SA1693F | 13314 | 0.00 | 38.50 | –233.14 | 1992/10/19 | 750–3,191 m | 4 | y |
| 1044 | SA1742A | 13721 | 0.00 | 41.10 | –240.91 | 1992/11/02 | 750–3,191 m | 4 | y |
| 1050 | SA1844B | 53 | 0.00 | 20.00 | –250.48 | 1992/12/01 | 750–3,191 m | 3b | y |
| 1051 | SA1861A | 54 | 3.60 | 20.20 | –254.12 | 1992/12/07 | 750–3,191 m | 3b | y |
| 1052 | SA1997A | 55 | 3.70 | 19.80 | –273.07 | 1993/01/13 | KLX02 | 4 | |
| 1053 | SA2025A | 56 | 0.00 | 40.40 | –277.76 | 1993/01/21 | KLX02 | 4 | |
| 1078 | SA2074B | 58 | 4.00 | 20.00 | –280.24 | 1993/02/05 | 750–3,191 m | 3b | y |
| 1079 | SA2109B | 13760 | 0.00 | 19.90 | –283.97 | 1993/02/15 | 750–3,191 m | 3b | y |
| 1080 | SA2142A | 2202 | 5.90 | 20.00 | –289.41 | 1993/12/02 | 750–3,191 m | 3b | y |
| 1083 | SA2192B | 60 | 5.80 | 20.00 | –295.87 | 1993/03/11 | 750–3,191 m | 3b | y |
| 1118 | SA2355B | 2227 | 5.90 | 20.00 | –318.07 | 1994/03/08 | 750–3,191 m | 3b | y |
| 1146 | SA2600B | 2225 | 5.80 | 19.20 | –345.00 | 1994/03/07 | 750–3,191 m | 3b | y |
| 1147 | SA2634B | 2219 | 6.00 | 20.40 | –349.66 | 1994/02/24 | 750–3,191 m | 3b | y |
| 1148 | SA2649A | 2220 | 5.80 | 19.85 | –352.14 | 1994/02/24 | 750–3,191 m | 3b 5 | y |
| 1149 | SA2663B | 2222 | 5.60 | 20.10 | –354.32 | 1994/02/24 | 750–3,191 m | 3b 5 | y |
| 1150 | SA2664A | 2221 | 5.80 | 20.40 | –353.84 | 1994/02/24 | 750–3,191 m | 3b | y |
| 1151 | SA2681B | 2216 | 5.60 | 17.30 | –357.90 | 1994/02/23 | 750–3,191 m | 3b | y |
| 1152 | SA2681A | 2215 | 5.70 | 21.80 | –356.32 | 1994/02/23 | 750–3,191 m | 3b | y |
| 1155 | SA2718A | 2238 | 5.80 | 20.30 | –361.61 | 1994/05/17 | 750–3,191 m | 3b 5 | y |
| 1156 | SA2734B | 2218 | 5.70 | 20.30 | –363.84 | 1994/02/23 | 750–3,191 m | 3b | y |
| 1157 | SA2768A | 2211 | 6.00 | 20.30 | –369.08 | 1994/02/14 | 750–3,191 m | 3b | y |
| 1158 | SA2768B | 2212 | 5.90 | 19.80 | –369.01 | 1994/02/14 | 750–3,191 m | 3b | y |
| 1173 | SA2834B | 2214 | 6.00 | 20.20 | –377.86 | 1994/02/14 | 750–3,191 m | 3b | y |
| 1207 | SM00352 | 297 | 0.00 | 32.60 | –90.30 | 1991/06/03 | 0–750 m | 4 | |
| 1208 | SM00451 | 13233 | 0.00 | 29.00 | –93.10 | 1991/06/03 | 0–750 m | 4 | |
| 1209 | SM00456 | 13465 | 0.00 | 29.00 | –100.71 | 1991/06/03 | 0–750 m | 4 | |
| 1210 | SM00457 | 277 | 0.00 | 29.00 | –100.92 | 1991/06/03 | 0–750 m | 4 | |

There are another 27 boreholes with only one sample in Data Set II (and none in Data Set I); the main reason is the incomplete major ions, but there are also 4 samples with a pH higher than 8.7, two samples with a high charge imbalance and one sample with a high percent of drilling water.

There are 22 boreholes in the second group (Table 6-6), 13 boreholes with 2 samples, 4 boreholes with 3 samples and 5 boreholes with 4 samples giving a total of 58 samples. From these 4 are Category 2, 23 are Category 3 (mainly because of the isotopes and the sample or time series), 10 are Category 3b (all of them with a grade of 4 in the isotopes), and finally, 21 samples are of Category 4. They were all sampled between 1991 (33 samples) and 1994 associated with the tunnel construction (26 during the 0-750 phase, and 32 during the 750-3,191 phase). In all the cases, the first sample taken in the borehole has been considered representative of initial conditions (22 samples).

There are 10 samples from these boreholes that have been categorised as Category 5 and are included in Data Set II (see Table 6-6) mainly because of the incomplete major ions, but also because of a high charge imbalance, high percent of drilling water and high pH. And there are 2 additional boreholes with two samples in Data Set II (SM00452 and SA00776B) that do not have samples in Data Set I.

The third group contains 22 boreholes (Table 6-7) with more than 4 samples (up to 25 in several boreholes) giving another 280 samples to Data Set I. Of these, one sample is Category 1, 105 samples are Category 2, 136 are Category 3 (mainly because of the isotopes and the sample or time series), 8 are Category 3b (all of them with a grade of 4 in the isotopes), and finally, 30 samples of Category 4. They were all sampled between 1991 and 2011. Samples taken during between 1991 and 1994 (106 samples) were associated with the tunnel construction (76 during the 0-750 phase, and 30 during the 750-3,191 phase). Then, the rest of the samples (174) were taken between 1995 and 2011 within the framework of the monitoring programme (GWCM; only one sample is associated with the LTDE project).

As for the previous group, in all the cases, the first sample taken in the borehole has been considered representative of initial conditions (22 samples).

There are 70 samples from these boreholes that have been categorised as Category 5 and are included in Data Set II (see Table 6-7) mainly because of the incomplete major ions, but also because of a high charge imbalance (in some samples with complete major ions). And there are 72 additional samples included in Data Set II (incomplete major ions) without samples in Data Set I.

**Table 6-6. List of probing boreholes with 2, 3 and 4 samples from the same section. They are sorted alphabetically by the ID code within each group. The table includes the information about the ID code of the borehole, the sample number, the section and its central elevation of the middle, the project which the sampling was associated with, the defined category, the indication of whether the sample is representative or not of the initial conditions and the ID number of the sample in Data Set I.**

| ID code | Sample no. | Elev. (m.a.s.l.) | Secup | Seclow | Project | Start date | Category | | Init. cond. | ID DS I |
|---|---|---|---|---|---|---|---|---|---|---|
| **Boreholes with 2 samples** | | | | | | | | | | |
| SA0271B | 13144 | –37.71 | 6.00 | 19.80 | 0–750 m | 1991/01/08 | 3b | | y | 843 |
| | 13167 | | | | | 1991/02/14 | 4 | | | 844 |
| SA0813A | 13253 | –112.65 | 5.70 | 19.00 | 0–750 m | 1991/08/05 | 3b | | y | 891 |
| | 13281 | | | | 750–3,191 m | 1991/11/05 | 4 | | | 892 |
| SA0831A | 328 | –115.05 | 6.00 | 20.00 | 0–750 m | 1991/08/08 | 3b | | y | 908 |
| | 13280 | | | | 750–3,191 m | 1991/11/05 | 4 | | | 909 |
| SA0831B | 327 | –116.16 | 4.60 | 19.50 | 0–750 m | 1991/08/08 | 3b | | y | 910 |
| | 13283 | | | | 750–3,191 m | 1991/11/06 | 4 | | | 911 |
| SA0850B | 13258 | –117.71 | 1.00 | 19.80 | 0–750 m | 1991/08/20 | 3 | | y | 912 |
| | 13278 | | | | 750–3,191 m | 1991/11/01 | 4 | | | 913 |
| SA0976B | 13271 | –134.14 | 1.00 | 10.50 | 750–3,191 m | 1991/10/15 | 3 | | y | 924 |
| | 13272 | | | | | 1991/10/16 | 4 | | | 925 |
| SA1062B | 13308 | –146.94 | 6.00 | 20.00 | 750–3,191 m | 1992/04/23 | 3 | 5 | y | 945 |
| | 2050 | | | | | 1992/12/02 | 3 | | | 946 |

| ID code | Sample no. | Elev. (m.a.s.l.) | Secup | Seclow | Project | Start date | Category | | Init. cond. | ID DS I |
|---|---|---|---|---|---|---|---|---|---|---|
| SA2175B | 2206 | –293.80 | 5.80 | 20.00 | 750–3,191 m | 1993/12/13 | 3 | | y | 1081 |
| | 2244 | | | | | 1994/05/30 | 3 | | | 1082 |
| SA2240B | 2175 | –301.52 | 5.70 | 19.80 | 750–3,191 m | 1993/09/28 | 3 | | y | 1084 |
| | 2204 | | | | | 1993/12/07 | 3 | | | 1085 |
| SA2273B | 2200 | –305.94 | 5.80 | 20.00 | 750–3,191 m | 1993/11/30 | 3 | 5 | y | 1110 |
| | 2245 | | | | | 1994/05/30 | 3 | | | 1111 |
| SA2289B | 2201 | –307.69 | 6.00 | 19.40 | 750–3,191 m | 1993/11/30 | 3 | | y | 1112 |
| | 2246 | | | | | 1994/05/30 | 3 | | | 1113 |
| SA2583A | 2223 | –343.49 | 5.70 | 20.00 | 750–3,191 m | 1994/03/07 | 3 | 5 | y | 1119 |
| | 2240 | | | | | 1994/05/18 | 3 | | | 1120 |
| SA2703A | 2237 | –358.56 | 5.70 | 19.60 | 750–3,191 m | 1994/05/17 | 3 | | y | 1153 |
| | 2217 | | | | | 1994/02/23 | 3 | | | 1154 |
| **Boreholes with 3 samples** | | | | | | | | | | |
| SA0289B | 13146 | –40.28 | 0.00 | 20.10 | 0–750 m | 1991/01/16 | 4 | 5 | y | 847 |
| | 13170 | | | | | 1991/02/20 | 4 | | | 848 |
| | 13171 | | | | | 1991/02/21 | 4 | | | 849 |
| SA0311B | 13157 | –43.27 | 6.00 | 19.00 | 0–750 m | 1991/01/31 | 3b | 5 | y | 855 |
| | 13188 | | | | | 1991/03/21 | 4 | | | 856 |
| | 13229 | | | | | 1991/05/29 | 4 | | | 857 |
| SA0452A | 13198 | –64.31 | 5.50 | 19.60 | 0–750 m | 1991/04/09 | 3b | 5 | y | 881 |
| | 273 | | | | 0–750 m | 1991/05/30 | 4 | 5 | | 882 |
| | 2260 | | | | 750–3,191 m | 1994/06/08 | 3 | | | 883 |
| SA0923A | 13279 | –128.38 | 6.00 | 20.00 | 750–3,191 m | 1991/11/01 | 3b | | y | 915 |
| | 2053 | | | | | 1992/12/02 | 2 | | | 916 |
| | 2075 | | | | | 1993/02/07 | 2 | | | 917 |
| **Boreholes with 4 samples** | | | | | | | | | | |
| SA0361B | 13173 | –51.56 | 6.00 | 19.00 | 0–750 m | 1991/02/27 | 3b | 5 | y | 871 |
| | 13193 | | | | | 1991/03/26 | 4 | | | 872 |
| | 13203 | | | | | 1991/04/24 | 4 | | | 873 |
| | 274 | | | | | 1991/05/30 | 4 | | | 874 |
| SA0327A | 13164 | –45.51 | 5.70 | 19.30 | 0–750 m | 1991/02/12 | 3b | 5 | y | 858 |
| | 13176 | | | | | 1991/02/28 | 4 | | | 859 |
| | 13191 | | | | | 1991/03/26 | 4 | | | 860 |
| | 13230 | | | | | 1991/05/29 | 4 | | | 861 |
| SA0344A | 13160 | –47.93 | 5.80 | 20.00 | 0–750 m | 1991/02/08 | 3b | 5 | y | 867 |
| | 13172 | | | | | 1991/02/27 | 4 | | | 868 |
| | 13192 | | | | | 1991/03/26 | 4 | | | 869 |
| | 13232 | | | | | 1991/05/29 | 4 | | | 870 |
| SA1614B | 2117 | –224.01 | 5.80 | 19.30 | 750–3,191 m | 1993/06/22 | 2 | 5 | y | 1003 |
| | 2149 | | | | | 1993/08/24 | 2 | 5 | | 1004 |
| | 2184 | | | | | 1993/09/28 | 3 | | | 1005 |
| | 2249 | | | | | 1994/06/06 | 3 | | | 1006 |
| SA2322A | 2174 | –312.58 | 6.00 | 20.10 | 750–3,191 m | 1993/09/28 | 3 | | y | 1114 |
| | 2205 | | | | | 1993/12/07 | 3 | | | 1115 |
| | 2226 | | | | | 1994/03/08 | 3 | | | 1116 |
| | 2243 | | | | | 1994/05/27 | 3 | | | 1117 |

**Table 6-7. Boreholes, sections (including their central elevation, m.a.s.l.) and samples corresponding to this object type (probing boreholes). As the boreholes were drilled during the tunnel construction, many of the samples correspond also to that time. However, only some of the borehole sections have been monitored (GWCM) over the years and this will be indicated when necessary. The column with comments indicate some specific information about the samples. Some abbreviations are used in this column in order to shorten the text: Cat for Category, DSI and DSII for Data Sets I and II, CI for charge imbalance, init. cond. for initial conditions and series for sample or time series.**

| Borehole section and vertical elevation (m) | Tot no | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **SA0158A** (–21.66) 6–19.70 | 5 | | | 1 | | 4 | | First strike selected as init. cond. and, except for one case, all of them are Category 3b due to the fact that they show a reasonably good quality except for the lack of isotopes (for the rest of the samples it means Cat. 4). |
| **SA0205A** (–28.26) 6–20 | 7 | | | 1 | 1 | 4 | 1 | |
| **SA0237B** (–32.74) 6–20 | 5 | | | 1 | 1 | 3 | | |
| **SA0311A** (–43.68) 5.7–19 | 7 | | | 1 | 1 | 3 | 2 | Sampling started in 1990 or 1991 (0–750 m) and the last sample was taken in 1994 during the construction of the second part of the tunnel. This last sample is best in category (3) due to more information about the isotopes. In all the cases Category 5 samples are due to incomplete major ions (one has a complete analysis but the CI is quite high). |
| **SA0327B** (–45.49) 5.7–19 | 6 | | | 1 | 1 | 3 | 1 | |
| **SA0435A** (–61.75) 6–22 | 5 | | | 1 | 1 | 3 | | |
| **SA0468**A (–67.5) 6–19.8 | 7 | | | 1 | 1 | 4 | 1 | |
| **SA0813B** (–112.9) 5.6–19.5 | 15 | | 4 | 8 | 1 | 2 | | Sampling started in 1991 and it has been monitored between 1995 and 1999 (GWCM). Good quality (better than the previous ones) except for the incomplete isotopes (Cats. 3 and 3b). |
| **SA0958B** (–133.17) 5–19.7 | 7 | | 2 | 2 | 1 | | 2 | Samples were taken during 1992–94 (750–3,191 m). All good quality except for the lack of isotopes in Cat.3b. Two Cat. 5 samples due to incomplete major ions. |
| **SA1009B** | 19 | | 10 | 7 | | | 2 | Two sections. 17 samples in DSI and 2 in DSII. Good quality samples except for the incomplete isotopes for Cat. 3. |
| (–139.45) 1.7–19.5 | 3 | | 3 | | | | | 3 very good samples taken during GWCM. |
| (–139.72) 6–19.5 | 16 | | 7 | 7 | | | 2 | 14 good samples except for the incomplete isotopes in Cat. 3. Sampling started with the tunnel construction in 1993 (750–3,191 m) and then this section has been monitored between 1995 and 2007 (GWCM).First strike was selected as init. cond. Two Cat. 5 samples due to incomplete major ions and high CI. |
| **SA1210A** (–167.92) 6–20.5 | 19 | | 4 | 1 | | | 14 | First strike selected as init. cond. Samples were taken during 1992–94 (750–3,191 m). All good quality. The 14 samples categorised as 5 because of incomplete major ions. |
| **SA1229A** (–171.26) 6–20.5 | 31 | | 9 | 8 | | | 14 | 7 samples were taken during 1992–94 (750–3,191 m) and then 11 during the monitoring programme (1995–2001). All good quality except for incomplete isotopes in Cat 3. 14 Cat. 5 due to incomplete major ions. |
| **SA1420A** | 30 | | | 25 | | | 5 | Two sections. 25 samples in DSI (all Cat. 3 due to the long sections) and 5 samples in DSII. |
| (–200.14) 1.15–50 | 6 | | | 2 | | | 4 | 2 reasonably good samples taken between 2009 and 2011 in the framework of the GWCM. Two Cat. 5 samples do not contain but a sulphide value; the other two, though having complete major ions, have a high CI. |
| (–200.56) 6–50 | 23 | | | 23 | | | 1 | 22 good samples except for the long section (Cat. 3) but the long time series compensates this weakness. Sampling started with the tunnel construction from 1992 to 1994 (8 samples and the first strike was selected as init. cond.) and then continued with the GWCM between 1995 and 2008. One Cat. 5 sample due to the high CI. |
| **SA1696B** (–232.62) 5.9–19.2 | 6 | | 4 | 2 | | | | Very good samples (except for the incomplete isotopes in the two Cat. 3 samples). First strike selected as init. cond. Samples were taken during 1992–94 (750–3,191 m). |
| **SA1730A** | 31 | | 18 | 10 | | | 3 | Two sections. 28 samples in DSI and 3 samples in DSII due to incomplete major ions. |
| (–236.65) 1.35–20 | 13 | | 9 | 2 | | | 2 | Good samples (only two of Cat. 3) taken between 2002 and 2011 in the framework of the GWCM. The two Cat. 5 samples do not contain but a sulphide value. |
| (–236.98) 5.6–20 | 18 | | 9 | 8 | | | 1 | Reasonably good samples except for the incomplete isotopes (Cat. 3). Sampling started with the tunnel construction (6 samples and the first strike was selected as init. cond., between1993 and 1994) and then continued with the GWCM between 1995 and 2001. One Cat. 5 sample due to incomplete major ions. |

| Borehole section and vertical elevation (m) | Tot no | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **SA1828B** (–249.48) 5.8–20 | 6 | | 3 | 2 | | | 1 | Quite good samples (except for the incomplete isotopes in the cat. 3 samples). First strike selected as init. cond. Samples were taken during 1992–94 (750–3,191 m). |
| **SA2074A** | 26 | | | 24 | | | 2 | Two sections. 24 samples in DSI (all Cat. 3 due to the long sections) and 2 samples in DSII. |
| (–281.3) 1.35–38.7 | 10 | | | 8 | | | 2 | Reasonably good samples (Cat. 3) taken between 2002 and 2011 in the framework of the GWCM. Two Cat. 5 samples due to incomplete major ions. |
| (–281.6) 6–38.7 | 16 | | | 16 | | | | Reasonably good samples except for the long section (graded as 3) but the long time series compensates this weakness. Sampling started with the tunnel construction (5 samples and the first strike was selected as init. cond., between1993 and 1994) and then continued with the GWCM between 1995 and 2001 (11 samples). |
| **SA2273A** | 33 | | 14 | 10 | | | 9 | Two sections. 24 samples in DSI and 9 samples in DSII (due to incomplete major ions). |
| (–305.59) 1.35–20 | 19 | | 8 | 2 | | | 9 | Good samples taken between 2002 and 2011 in the framework of the GWCM. Five of the Cat. 5 samples do not have any data, one has only data for sulphide and the other 3 contain data for chloride, bicarbonate, sulphate and one of them also for $\delta^{18}O$, $\delta^{2}H$ and $^{3}H$. |
| (–305.94) 5.8–20 | 14 | | 6 | 8 | | | | Quite good samples except for the incomplete isotopes in the Cat 3 samples. Sampling started with the tunnel construction (3 samples between1993 and 1994, and the first strike was selected as init. cond.) and then continued with the GWCM between 1995 and 2001 (11 samples). |
| **SA2600A** | 28 | | 15 | 10 | | | 3 | Two sections. 25 samples in DSI and 3 in DSII (due to incomplete major ions). |
| (–344.6) 1.35–19.4 | 13 | | 9 | 2 | | | 2 | Good samples taken between 2002 and 2011 in the framework of the GWCM. The two Cat. 5 samples do not have but a data for sulphide. |
| (–345) 5.8–19.4 | 15 | | 6 | 8 | | | 1 | Good samples except for the incomplete isotopes in the cat 3 samples. Sampling started with the tunnel construction (3 samples in 1994, and the first strike was selected as init. cond.) and then continued with the GWCM between 1995 and 2001 (11 samples). One Cat. 5 sample due to incomplete major ions. |
| **SA2783A** | 15 | | 5 | 7 | | 2 | 1 | Two sections. 14 samples in DSI and 1 sample in DSII (incomplete major ions). |
| (–370.8) 1.35–19.9 | 1 | | | | | 1 | | Sample taken in 2002 GWCM. |
| (–371.33) 5.8–19.9 | 14 | | 5 | 7 | | 1 | 1 | Good samples except for the incomplete isotopes in Cats 3 and 4. Sampling started with the tunnel construction (3 samples in 1994, and the first strike was selected as init. cond.) and then continued with the GWCM between 1995 and 2000 (10 samples). |
| **SA2880A** | 19 | | 10 | | 5 | | 4 | Two sections. 15 samples in DSI and 4 in DSII due to incomplete major ions or a high Cl. All correspond to GWCM. |
| (–384.09) 0–19.9 | 7 | | 2 | 2 | | | 3 | Good samples taken between 2008 and 2011. Cat. 5 samples only contains some data for chloride and sulphide. |
| (–384.71) 6–19.9 | 12 | | 8 | 4 | | | | Good samples except for the incomplete isotopes in Cat 3 samples. Sampling between 1995 and 2007. |
| **SA3045A** | 23 | 1 | 7 | 8 | | 2 | 5 | 4 sections. 18 samples in DSI and 5 in DSII (incomplete major ions). All taken during the monitoring program GWCM except one sample associated with project F79 LTDE (Cat. 4). |
| (–407.27) 0–20.7 | 9 | | | 6 | | 1 | 2 | Samples taken between 1995 and 1999. Cats 3 and 4 due to long sections, in some cases incomplete ions or isotopes. |
| (–406.66) 6–8 | 9 | 1 | 4 | 1 | | 1 | 2 | Good samples except for the incomplete isotopes in the Cat. 3 samples. Sampling between 2001 and 2011. One of the samples taken in 2003 was associated with project F79 LTDE. Cat. 5 samples only contains some data for Cl and S(-II). |
| (–407.82) 6–20 | 1 | | 1 | | | | | This section includes the previous one. Very good quality sample taken in 2000. |
| (–408.09) 9–20.7 | 4 | | 2 | 1 | | | 1 | Good samples. Cat. 5 sample only contain data for sulphide. |

## 6.3 Other boreholes drilled during the construction phase

### 6.3.1 Description

This group of boreholes includes those that were drilled during the tunnel construction phase (from 1991 until 1995). In general, investigation boreholes were drilled for certain purposes and studied according to programmes specially designed for each borehole. However, a main general purpose was to characterise the far-field rock volumes 20–400 m from the tunnel. These boreholes were normally core or percussion drilled and could also be considered as extended probe holes through fracture zones etc (Almén and Stenberg 2005, Stanfors et al. 1997a).

### 6.3.2 Results from quality assessment

The total number of boreholes in this group is 70 (33 percussion and 37 cored drilled boreholes) and the total number of samples taken from them and included in Data Sets I and II is 665. However, 210 of these samples have been categorised as Category 5 and, therefore, they are included in Data Set II. 34 of them correspond to 21 boreholes whose samples are all Category 5 and there are no samples from these boreholes in Data Set I. They are listed in Table 6-8 together with the number of samples taken in each borehole. The other 176 Category 5 samples correspond to boreholes that have other good quality samples stored in Data Set I; these samples will be considered in the corresponding borehole description (Tables 6-10 to 6-12).

The list of the 49 boreholes included in Data Set I (with some samples in Data Set II) is shown in Table 6-9 separated into two columns representing percussion and cored boreholes. The main studies/investigations in each borehole are also indicated in the table (Stanfors et al. 1997a).

As shown for the probing boreholes, the boreholes in this group have also been separated into three groups depending on the number of samples that have been taken over the time. There are 16 boreholes with 1 sample (listed in Table 6-10), 13 boreholes with between 2 to 4 samples (Table 5-11), and 20 boreholes with more than 4 samples (Table 6-12).

There are 16 boreholes with *only one sample in Data Set I (Table 6-10)*. 14 of them were sampled only once and 2 have another sample in Data Set II (HA1273 has 2 samples and KA2858 has 1). From the total of 19 samples, 3 of them have been categorised as Cat. 3b, 13 as Cat. 4 and another 3 as Category 5 (these in Data Set II). Samples in this group were taken between 1991 and 1995 and except for the latest one that corresponds to the project Select, the rest of the samples are associated with projects 0–750 m and 750–3,191 (the construction of the first and second part of the tunnel). There are 3 samples in this group that have been considered representative of the initial conditions in the system (the ones that were subsequently categorised as 3b). As indicated before, and as shown in the column with the categories in Table 6-10, apart from the samples just mentioned included in Data Set I, there are 3 samples taken in some of these boreholes that belong to Category 5 (indicated in Table 6-10) due to the incomplete major ions. Finally, there are another 14 boreholes with only one sample in Data Set II (14 additional Cat. 5 samples due to the incomplete major ions) and none in Data Set I.

**Table 6-8. Boreholes in this group of objects whose samples are only included in Data Set II. The number of samples taken from them are indicated between brackets. There are 16 percussion drilled and 5 cored drilled boreholes.**

| | | | |
|---|---|---|---|
| HA0992F (1) | HA1145F (1) | HA2265A (1) | KA1754A (1) |
| HA1048A (1) | HA1274A (2) | HA2713A (1) | KA2048B (3) |
| HA1073F (1) | HA1290F (2) | HA2743B (1) | KC0045F (6) |
| HA1086F (1) | HA1292F (1) | HA2778B (1) | |
| HA1103F (1) | HA1405B (1) | KA0747A (3) | |
| HA1130B (2) | HA2198B (1) | KA1751A (2) | |

**Table 6-9. List of the boreholes included in this object type (construction phase and principal studies/investigations; from Stanfors et al. 1997a) and whose samples are in Data Set I and II. The list is sorted alphabetically by the ID code. There are a total of 49 boreholes, 17 were percussion drilled and 32 cored drilled.**

| Borehole ID code | Principal Studies and investigations |
|---|---|
| **Percussion boreholes** | |
| HA0982B | Grouting of NE-3 |
| HA0991I | |
| HA1272A | Passage of NE-1 |
| HA1273A | |
| HA1275A | |
| HA1276A | |
| HA1278A | |
| HA1283B | |
| HA1284B | |
| HA1285B | |
| HA1286B | |
| HA1327B | |
| HA1330B | |
| HA1684B | Facture zones and inflow mapping* |
| HA1749A | |
| HA2780A | |
| HD0025A | |

| Borehole ID code | Principal Studies and investigations |
|---|---|
| **Cored boreholes** | |
| KA0483A | Redox |
| KA0531B | Blasting damage invest |
| KA0545B | |
| KA0552B | |
| KA0575A | Passage of fracture zone |
| KA0644B | |
| KA0667B | |
| KA0745B | |
| KA1061A | Passage of NE-1 |
| KA1131B | |
| KA1639A | Invest. of fracture zones and inflow mapping* |
| KA1750A | |
| KA1755A | |
| KA2050A | Degassing of gw and two-phase flow** |
| KA2162B | |
| KA2511A | |
| KA2512A | |
| KA2598A | |
| KA2858A | Fracture zones and inflow mapping* |
| KA2861A | |
| KA2862A | |
| KA3005A | |
| KA3010A | |
| KA3067A | |
| KA3068A | |
| KA3105A | |
| KA3110A | |
| KA3191F | Comp. study TBM |
| KA3385A | Comp. study TBM, F58 RNR |
| KR0012B | Redox |
| KR0013B | Redox |
| KR0015B | Redox |

* Classification and characterisation of water-conducting features ~ 690 to 2,940 m.
Supplementary investigations of fracture zones ~ 1,280 to 2,840 m.
Supplementary inflow mapping ~ 1,584 to 2,496 m.
Definition and characterization of N-S fracture system between tunnel sections 1,600 to 2,400 m.

** Groundwater degassing and two-phase flow: Pilot hole test Bubble pressure estimates were calculated from earlier gas contents measurements in KA2511A and KA2598A.

**Table 6-10. List of the 16 boreholes included in this group of objects with only one sample taken (or one sample kept in Data Set I). The table includes the information about the ID number of the sample in Data Set I, the ID code of the borehole, the sample number, the section and the elevation of the middle, the sampling data, the project which the sampling was associated with, the indication of whether the sample is representative or not of the initial conditions and the defined category.**

| ID DS I | ID code | Sample no. | Secup | Seclow | Elev. (m.a.s.l.) | Date | Project | Initial cond. | Category |
|---|---|---|---|---|---|---|---|---|---|
| 2 | HA0982B | 2279 | 0.00 | 2.50 | –133.48 | 1994/09/05 | 0–750 m | | 4 |
| 3 | HA0991I | 137 | 0.00 | 14.50 | –125.36 | 1992/01/31 | 0–750 m | | 4 |
| 4 | HA1272A | 13296 | 0.00 | 32.00 | –176.18 | 1992/03/14 | 750–3,191 m | | 4 |
| 5 | HA1273A | 13299 | 0.00 | 23.00 | –172.07 | 1992/03/15 | 750–3,191 m | | 4 5(2) |
| 8 | HA1276A | 13298 | 0.00 | 24.50 | –179.23 | 1992/03/15 | 750–3,191 m | | 4 |
| 9 | HA1278A | 51 | 0.00 | 29.00 | –174.57 | 1992/11/15 | 750–3,191 m | | 4 |
| 10 | HA1283B | 13297 | 0.00 | 35.50 | –178.99 | 1992/03/14 | 750–3,191 m | | 4 |
| 11 | HA1284B | 13295 | 0.00 | 38.50 | –180.00 | 1992/03/13 | 750–3,191 m | | 4 |
| 12 | HA1285B | 126 | 0.00 | 41.50 | –180.41 | 1992/03/14 | 750–3,191 m | | 4 |
| 13 | HA1286B | 127 | 0.00 | 40.50 | –180.46 | 1992/03/14 | 750–3,191 m | | 4 |
| 22 | HA1684B | 64 | 1.60 | 25.00 | –230.30 | 1993/03/25 | 750–3,191 m | | 4 |
| 23 | HA1749A | 63 | 5.80 | 25.00 | –239.10 | 1993/03/25 | 750–3,191 m | | 4 |
| 57 | KA0531B | 13222 | 1.00 | 6.00 | –73.25 | 1991/05/24 | 0–750 m | y | 3b |
| 58 | KA0545B | 13219 | 1.25 | 6.00 | –75.23 | 1991/05/23 | 0–750 m | y | 3b |
| 59 | KA0552B | 13221 | 1.05 | 6.00 | –76.19 | 1991/05/23 | 0–750 m | y | 3b |
| 212 | KA2858A | 2298 | 39.77 | 40.77 | –382.35 | 1995/03/10 | Select | | 4 5 |

There are 13 boreholes in the second group (Table 6-11), 6 boreholes with 2 samples, 4 boreholes with 3 samples and 3 boreholes with 4 samples giving a total of 36 samples. From them 1 sample is Category 2, 17 are Category 3, 6 are Category 3b, and 12 samples are Category 4 (the more or less incomplete set of isotopes is the main reason for the lower categories). Eight of these samples have been considered representative of initial conditions. Apart from these samples, there are another 20 samples taken from some of these boreholes that have been categorised as Category 5 (mainly because of the incomplete major ions, but two of them, despite having a complete chemical analyses, they are discarded due to a high charge imbalance and another one due to a high pH value) and are included in Data Set II.

Samples in this group were all taken between 1991 and 2011 and they were associated with different investigations after the tunnel construction (REX, 2-phase flow, LTDE, Colloid, GWCM, Select and TBM).

There are 20 boreholes in the third group (Table 6-12) with more than 4 samples giving a total of 403 samples in Data Set I. From them, 6 are Category 1, 171 samples are Category 2, 102 are Category 3 (mainly because of the incomplete isotopes and the long sections), 3 are Category 3b (all of them with a grade of 4 in the isotopes), and finally, 121 samples of Category 4. They were all sampled between 1991 and 2011. Samples taken between 1991 and 1993 (135 samples) were associated with the tunnel construction (15 during the 0–750 phase, and 18 during the 750–3,191 phase) and with the project REDOX (135 samples). Then, the rest of the samples (235) were taken between 1995 and 2011 most of them associated with the monitoring program (GWCM) and only 23 of them associated with other investigations (TRUE and True Block Scale, RNR, LTFE, Backfill & Plug projects, Redox and Selec). There are 153 samples from these boreholes that have been categorised as Category 5 and are included in Data Set II (see Table 6-12) mainly because of the incomplete major ions and in some cases a high percent of drilling water or a high charge imbalance (in some samples with complete major ions), only one sample was discarded because of a high pH value. And there are 6 additional samples from borehole KC0045F, included in Data Set II (incomplete major ions) without samples in Data Set I.

**Table 6-11. List of the boreholes included in this group of objects with 2, 3 and 4 samples for the same section. They are sorted alphabetically by the ID code inside each group. The table includes the information about the ID code of the borehole, the sample number, the section and the elevation of the middle, the project which the sampling was associated with, the sampling date, the defined category (including the number of samples corresponding to Cat. 5, between brackets), the indication of whether the sample is representative or not of the initial conditions and the ID number of the sample in Data Set I.**

| ID code | Sample no. | Elev. (m.a.s.l.) | Secup | Seclow | Project | Start date | Category | | Init. cond. | ID DS I |
|---|---|---|---|---|---|---|---|---|---|---|
| **Boreholes with 2 samples** | | | | | | | | | | |
| HA1275A | 128 | –178.83 | 0.00 | 29.50 | 750–3,191 m | 1992/03/14 | 4 | | | 6 |
| | 13307 | | | | | 1992/04/09 | 4 | | | 7 |
| KA0483A | 1800 | –75.09 | 40.00 | 90.00 | 0–750 m | 1991/03/12 | 3 | | y | 55 |
| | 13183 | | | | | 1991/03/13 | 4 | | y | 56 |
| KA0667B | 13265 | –92.01 | 2.50 | 10.03 | 0–750 m | 1991/09/21 | 3b | 5(2) | y | 75 |
| | 13266 | –92.63 | 10.00 | 20.21 | | 1991/09/21 | 3b | | y | 76 |
| KA2598A | 6773 | –421.73 | 0.00 | 300.00 | GWCM | 2005/10/18 | 4 | 5(2) | | 210 |
| | 14957 | | | | | 2009/10/07 | 4 | | | 211 |
| KA3068A | 6013 | –407.94 | 0.00 | 16.85 | F79 LTDE | 2003/04/10 | 4 | 5 | | 262 |
| | 20967 | | | | | 2011/10/07 | 3 | | | 263 |
| KA3191F/1 | 2247 | –444.32 | 165.00 | 180.00 | TBM | 1994/06/03 | 3 | 5(2) | | 283 |
| | 2248 | –449.20 | 193.90 | 208.90 | | 1994/06/04 | 3 | | | 284 |
| **Boreholes with 3 samples** | | | | | | | | | | |
| HA1330B | 3465 | –183.13 | 6.00 | 32.50 | GWCM | 2001/10/15 | 3 | | | 19 |
| | 3814 | | | | | 2002/09/26 | 3 | | | 20 |
| | 6367 | | | | | 2004/09/27 | 3 | | | 21 |
| KA1750A | 2140 | –237.22 | 4.40 | 5.40 | 750–3,191 m | 1993/08/10 | 2 | 5(2) | | 116 |
| | 2169 | | | | | 1993/09/27 | 3 | 5 | | 117 |
| | 2179 | | | | | 1993/09/29 | 3 | | | 118 |
| KA3010A/2 | 2293 | –402.45 | 0.00 | 60.66 | Select | 1994/12/14 | 3 | 5 | | 244 |
| | 2302 | –400.84 | 8.56 | 15.06 | Select | 1995/03/10 | 3 | 5 | | 242 |
| | 20963 | –400.84 | 8.56 | 15.06 | GWCM | 2011/10/06 | 3 | | | 243 |
| KA3105A/1 | 2294 | –416.48 | 0.00 | 68.95 | Select | 1994/12/16 | 3 | 5(3) | | 264 |
| | 2304 | –415.59 | 22.51 | 24.51 | Select | 1995/03/10 | 3 | | | 265 |
| | 20970 | –415.59 | 22.51 | 24.51 | GWCM | 2011/10/11 | 3 | | | |
| **Boreholes with 4 samples** | | | | | | | | | | |
| KA0745B | 13267 | –102.59 | 2.50 | 10.00 | 0–750 m | 1991/09/22 | 3b | | y | 78 |
| | 13270 | –102.77 | 3.25 | 19.75 | | 1991/09/29 | 3b | | y | 80 |
| | 13268 | –102.90 | 10.00 | 20.03 | | 1991/09/22 | 3b | | y | 77 |
| | 13269 | –103.94 | 40.00 | 50.01 | | 1991/09/23 | 3b | | y | 79 |
| KA2512A/1 | 2291 | –336.41 | 0.00 | 37.27 | F60 2-phase flow | 1994/12/13 | 3 | | | 176 |
| | 2391 | –336.41 | 0.00 | 37.27 | GWCM | 1997/03/11 | 3 | | | 177 |
| | 6904 | –336.41 | 0.00 | 37.27 | F91 COLLOID | 2006/05/19 | 4 | | | 178 |
| | 2515 | –337.28 | 34.00 | 37.27 | GWCM | 1998/03/11 | 4 | | | 179 |
| KA2861A/1 | 2517 | –379.29 | 0.00 | 8.52 | GWCM | 1998/03/13 | 4 | | | 213 |
| | 2474 | –379.67 | 8.69 | 9.34 | F57 REX | 1998/02/04 | 4 | 5(2) | | 214 |
| | 2577 | –379.67 | 8.69 | 9.34 | F57 REX | 1998/07/07 | 4 | 5 | | 215 |
| | 2677 | –379.67 | 8.69 | 9.34 | F57 REX | 1998/10/29 | 4 | | | 216 |

**Table 6-12. Boreholes, sections (including the elevation, m.a.s.l., of the middle of the section) and samples corresponding to this object type (construction phase and principal studies/investigations). As the boreholes were drilled during the tunnel construction, many of the samples correspond also to that time. However only some of the borehole sections have been monitored (GWCM) over the years and this will be indicated when necessary. The column with comments indicate some specific information about the samples. Some abbreviations are used in this column in order to shorten the text: Cat for Category, DSI and DSII for Data Sets I and II, CI for charge imbalance, init. cond. for initial conditions and series for sample or time series.**

| Borehole section and vertical elevation (m) | Tot. no. | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **HA1327B**<br>(–182.91) 0–29.5 | 6 | | | 5 | | | 1 | Samples taken in 1992 and 1993 associated with 750–3,191 m. An additional sample was taken in 2004 in ÄFS – svavel och multielement. Cat. 3 samples due to the long section. One Cat. 5 sample due to incomplete major ions (Cl missed). |
| **HA2780A** | 18 | | | 8 | | 1 | 9 | Several section lengths. 9 samples in DSI and 9 in DSII (due to incomplete major ions; 5 samples have no data at all).<br>Cat. 3 samples due to the long section. Samples in DSI associated with the monitoring program (GWCM), samples in DSII are also associated with F91 Colloid and F4P1 Kemimonitering. |
| (–380.41) 0–43.3 | 11 | | | 5 | | | 6 | |
| (–380.74) 1.2–43.3 | 6 | | | 3 | | | 3 | |
| (–387.03) 24–43.3 | 1 | | | | | 1 | | |
| **HD0025A**<br>(–415.76) 0–15 | 18 | | 9 | 2 | | | 7 | 11 good quality samples in DSI associated with GWCM and 7 in DSII (mainly due to incomplete major ions but there are 4 without any data) associated also to Select, F4P1 Kemimonitering, F61 Backfill&Plug and F63 Prototype. |
| **KA0575A**<br>(–85.75 to –96.5)<br>0–160 | 9 | | | | 1 | 5 | 3 | Each sample different section. 6 samples in DSI (considered representative of init. cond.) and 3 in DSII (1 with incomplete major ions, 1 with a high charge imbalance and 1 with a high pH value). Cat 4 samples due to the incomplete isotopes and inadequate series. Sampling associated with the tunnel construction. |
| **KA0644B**<br>(–91.72 to –100)<br>20–119.7 | 11 | | | | 2 | 7 | 2 | Different sections quite long (longer than 20 m). 9 samples in DSI (all considered init. cond.) and 2 in DSII (due to incomplete major ions and high percent of Drilling water). Cat 4 samples due to the incomplete isotopes and inadequate series. Sampling associated with the tunnel construction (750–3,191 m). |
| **KA1061A**<br>(–143.98) 0–208.5 | 23 | | | | | 19 | 4 | 19 samples in DSI (all Cat. 4 due to the section length) and 4 in DSII (due to incomplete major ions and to high charge imbalance). 3 samples associated with the tunnel construction (750–3,191 m) and then to GWCM. One Cat. 5 sample also associated with F4P1 Kemimonitering. |
| **KA1131B**<br>(–178.85) 0–203.1 | 9 | | | | | 9 | | All the samples are Cat. 4 due to the long sections. 1 sample associated with the tunnel construction (750–3,191 m) and the rest to GWCM and F91 Colloid. |
| **KA1639A** | 10 | | 4 | 3 | | | 3 | 2 sections. 7 good quality samples in DSI and 3 in DSII (due to incomplete major ions, 2 of them with no data). All the samples are associated with the tunnel construction (750–3,191 m). |
| (–223.2) 13.4–14.4 | 4 | | 2 | 2 | | | 1 | |
| (–222.6) 15.4–25.9 | 3 | | 2 | 1 | | | 2 | |
| **KA1755A** | 33 | | | 19 | | 1 | 13 | 3 Sections. 20 samples in DSI and 13 in DSII (mainly due to incomplete major ions, 4 of them without data). Except for one Cat. 4 sample, in DSI the rest of the samples are Cat. 3, mainly due to the lenght of the section. Samples in DSI are associated with the GWCM, but in DSII they are also associated with the tunnel construction (750–3,191 m) and to F91 Colloid. |
| (–235.5) 6–87 | 8 | | | 3 | | | 5 | |
| (–279.9) 88–160 | 23 | | | 16 | | | 7 | |
| (–334.6) 231–320.5 | 2 | | | | | 1 | 1 | |
| **KA2050A** | 15 | | | 12 | | | 3 | 2 sections. 12 Cat. 3 samples in DSI associated with the GWCM, and 3 in DSII (due to incomplete major ions) associated with the tunnel construction (750–3,191 m). Cat. 3 due to the length of the sections. |
| (–378.62) 102–154 | 6 | | | 3 | | | 3 | |
| (–422.81) 155–211.6 | 9 | | | 9 | | | | |
| **KA2162B** | 22 | | | 15 | | 3 | 4 | 4 sections. 18 samples in DSI associated with the tunnel construction (three Cat. 4 samples due to long section and inadequate series) and to the monitoring GWCM (15 Cat. 3 samples, due to the long sections).<br>4 samples in DSII (mainly due to incomplete major ions except one with a complete analysis but a high charge imbalance) associated with the tunnel construction and to the F4P1 Kemimonitering. |
| (–300.03) 0–76.7 | 1 | | | | | 1 | | |
| (–306.11) 0–127.77 | 1 | | | | | 1 | | |
| (–313.61) 0–180 | 1 | | | | | 1 | | |
| (–353.21) 201.5–288 | 19 | | | 15 | | | 4 | |

| Borehole section and vertical elevation (m) | Tot. no. | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **KA2511A** | 35 | | 4 | 5 | | 5 | 21 | Several sections (some of them short). 14 samples in DSI associated with the monitoring program (GWCM) and 21 in DSII (all due to incomplete major ions, 10 of them only have Cl). Category 5 samples (DSII) are associated with the tunnel construction, the F56 TRUE Block Scale and the CWCM. |
| (–365.02) 52–54 | 22 | | | | | 2 | 20 | |
| (–391.22) 92–109 | 2 | | | | | 2 | 1 | |
| (–394.51) 103–110 | 4 | | 4 | | | | | |
| (–404.41) 111–138 | 5 | | | 5 | | | | |
| (–420.87) 139–170 | 1 | | | | | 1 | | |
| **KA2862A** | 22 | | 10 | 2 | | 2 | 8 | 3 sections. 14 samples in DSI associated with the monitoring program (GWCM) and one of the associated with F61 Backfill&Plug. Categories 3 and 4 due to the incomplete isotopes (the samples series are adequate). Eight Category 5 samples in DSII (due to incomplete major ions) and associated with the project F57 REX and the GWCM. |
| (–380.63) 0–16 | 14 | | 4 | 2 | | | 8 | |
| (–380.87) 3.4–16 | 1 | | 1 | | | | | |
| (–381.15) 7.4–16 | 7 | | 5 | | | 2 | | |
| **KA3005A** | 19 | | 1 | 1 | | 5 | 12 | 4 sections (three of them very short). 7 samples in DSI but not very good quality due to the inadequate series or the incomplete isotopes. Twelve samples in DSII (all due to incomplete major ions, some of them only Cl or S(-II) except one with a high percent of drilling water. Samples in DSI are associated with Select, F83 TRUE-1 and GWCM; in DSII there is also a sample associated with Select and another one associated with F91 Colloid. One Cat. 5 sample due to the high percent of drilling water |
| (–402.15) 0–58.1 | 12 | | | | | 1 | 11 | |
| (–402.79) 36.9–37.9 | 1 | | | | | 1 | | |
| (–403.38) 44.8–45.8 | 4 | | 1 | 1 | | 1 | 1 | |
| (–403.61) 46.8–50 | 2 | | | | | 2 | | |
| **KA3067A** | 9 | | | 2 | | 4 | 3 | 4 sections (2 of them short). 6 samples in DSI but not very good quality due to length of the section or the incomplete isotopes or the inadequate series. These samples are associated with Select, F83 TRUE-1, F79 LTDE and GWCM. There are 3 Cat. 5 samples in DS2 (incomplete major ions). |
| (–410.24) 0–40 | 1 | | | | | 1 | | |
| (–409.97) 6.5–27 | 1 | | | | | 1 | | |
| (–410.98) 28.29.5 | 6 | | | 2 | | 1 | 3 | |
| (–411.26) 30.5–33.5 | 1 | | | | | 1 | | |
| **KA3110A** | 17 | | | | | | 1 | 2 sections (the first one covers the whole length of the borehole and only 1 sample, the other is shorter and contain the rest of the samples). 16 good quality samples in DSI (except for the first one) and 1 in DSII (incomplete major ions).<br>Sampling was associated with Select and then to GWCM. |
| (–414.94) 0–26.8 | 1 | | | | | 1 | | |
| (–415.91) 20–26.8 | 16 | 2 | 11 | 2 | | | 1 | |
| **KA3385A** | 27 | | | | | | | 3 sections (the first one covering the whole length of the borehole and only 1 sample, the second with 2 samples and the third much shorter with the rest of the samples). 18 good quality samples in DSI except for the three samples associated with the two first sections. There are 9 sample in DS 2 (incomplete major ions, four of them with no data, one only with S(-II)). Sampling was associated with F58 RNR, GWCM and F56 TRUE Block Scale. Some Cat. 5 samples were also associated with F91 Colloid. |
| (–447.19) 0–34.2 | 1 | | | | | 1 | | |
| (–447.33) 7–31 | 2 | | | | | 2 | | |
| (–448.35) 32–34.2 | 15 | | 12 | 3 | | | 9 | |
| **KR0012B** | 95 | 2 | 40 | 7 | | 25 | 21 | 3 very short sections. Good quality samples in general. 74 samples in DSI and 21 in DSII (mainly due to incomplete major ions but 3 of them due to a high percent of drilling water and another one due to a high charge imbalance). Most of the samples are associated with the Redox project and then to the GWCM (one Cat. 5 sample was associated with the F4P1 Kemimonitering). |
| (–69.13) 1.2–10.6 | 2 | | | | | 2 | | |
| (–69.16) 4–10.6 | 11 | | 6 | | | | 5 | |
| (–69.17) 5–10.6 | 82 | 2 | 34 | 7 | | 23 | 16 | |
| **KR0013B** | 86 | 2 | 40 | 6 | | 19 | 19 | 3 short sections (the first one covering the whole length of the borehole and only 1 sample, the second and the third shorter with the rest of the samples). Good quality samples. Cat. 4 samples due to the inadequate series. 67 samples in DSI associated with the Redox project and then to the monitoring GWCM. There are 19 samples in DSII (mainly due to incomplete major ions except for three of them due to a high charge imbalance and a high percent of drilling water). |
| (–69.19) 1.2–16.9 | 1 | | | | | 1 | | |
| (–69.23) 6–16.9 | 11 | | 6 | 1 | | | 4 | |
| (–69.24) 7–16.9 | 74 | 2 | 34 | 5 | | 18 | 15 | |
| **KR0015B** | 73 | | | | | | 11 | 3 sections slightly longer than the previous borehole (the first one covers the whole length of the borehole and only 1 sample, the second and the third shorter with the rest of the samples). Quite good quality samples. Cat. 4 samples due to the inadequate series. 62 samples in DSI and 11 in DSII (mainly due to incomplete major ions except 3 of them with a high charge imbalance). All of them associated with the Redox Project and to the monitoring program GWCM (one Cat. 5 sample was associated with the F4P1 Kemimonitering). |
| (–69.35) 1.2–30.3 | 2 | | | | | 2 | | |
| (–69.44) 10.8–30.3 | 10 | | 7 | 3 | | | | |
| (–69.51) 19.8–30.3 | 61 | | 33 | 7 | | 10 | 11 | |

## 6.4 Project boreholes

### 6.4.1 Description

Under this object type, boreholes drilled after the tunnel construction for different purposes/projects are included. We have differentiated two groups here:

- Group A) boreholes corresponding to specific projects in which the samples were not disturbed; then, all or part of their samples were considered suitable for the hydrogeochemical study and therefore they undergone the categorisation process and were finally included in Data Sets I or II.
- Group B) boreholes associated with projects that disturbed the system with specific experiments; groundwaters sampled during these experiments were not considered suitable for the hydrogeochemical study of the system and, therefore, they were included in Data Set IV without any additional treatment.

### 6.4.2 Boreholes, borehole sections and samples in Data Sets I and II (Group A)

Table 6-13 lists the boreholes from which some samples were taken in the framework of specific research projects, but these samples have been considered suitable for modelling purposes and, therefore, they are also included in Data Sets I and II. They will be described in the same way as the previous object above.

**Table 6-13. List of the 54 project boreholes (from the operational phase), with samples included in Data Sets I and II. The main studies/investigations in each borehole are also indicated in the table (Stanfors et al. 1997a). Groundwater monitoring (GWCM) have also been performed in some of the boreholes at a later stage.**

| Borehole | Project | Borehole | Project |
|---|---|---|---|
| DA1619A02 | KBS-3, KBS-®3H | KA3566G01 | F63 PROTOTYPE |
| HG0038B01 | F62 LOT | KA3566G02 | F63 PROTOTYPE |
| HMJ01 | F4P1 Kemimonitering | KA3572G01 | F63 PROTOTYPE |
| KA2051A01 | TUDP002 Utbyggnad Äspö | KA3573A | F63 PROTOTYPE |
| KA2169A01 | F83 TRUE-1 | KA3590G01 | F63 PROTOTYPE |
| KA2169A02 | F83 TRUE-1 | KA3590G02 | F63 PROTOTYPE |
| KA2169A03 | F83 TRUE-1 | KA3593G | F63 PROTOTYPE |
| KA2423A01 | F83 TRUE-1 | KA3600F | F63 PROTOTYPE |
| KA2423A03 | F83 TRUE-1 | KF0051A01 | F80P1 Matrix |
| KA2563A | F56 TRUE Block Scale | KF0066A01 | F80P1 Matrix |
| KA2865A01 | Select-2 | KG0021A01 | F63 PROTOTYPE |
| KA3007A01 | TUDP002 Utbyggnad Äspö | KG0048A01 | F63 PROTOTYPE |
| KA3065A02 | F79 LTDE | KI0023B | F56 TRUE Block Scale |
| KA3065A03 | F79 LTDE | KI0025F | F56 TRUE Block Scale |
| KA3386A02 | F73P3 Mini Can | KI0025F02 | F56 TRUE Block Scale |
| KA3386A03 | F73P3 Mini Can | KI0025F03 | F56 TRUE Block Scale |
| KA3386A04 | F73P3 Mini Can | KJ0044F01 | F58 RNR |
| KA3386A05 | F73P3 Mini Can | KJ0050F01 | Microbe |
| KA3386A06 | F73P3 Mini Can | KJ0052F01 | Microbe |
| KA3510A | F56 TRUE Block Scale | KJ0052F02 | F58 RNR |
| KA3539G | F63 PROTOTYPE | KJ0052F03 | Microbe |
| KA3542G01 | F63 PROTOTYPE | KXTT1 | F83 TRUE-1 |
| KA3542G02 | F63 PROTOTYPE | KXTT2 | F83 TRUE-1 |
| KA3545G | F63 PROTOTYPE | KXTT3 | F83 TRUE-1 |
| KA3548A01 | F63 PROTOTYPE | KXTT4 | F83 TRUE-1 |
| KA3554G01 | F63 PROTOTYPE | KXTT5 | F83 TRUE-1 |
| KA3554G02 | F63 PROTOTYPE | KZ0027A | F64 Demoförvar |

The total number of boreholes in this group is 54 (Table 6-13) and the number of samples taken from them and included in Data Sets I and II is 573. Data Set I includes 369 of these samples which correspond to 10 boreholes with single samples, 17 boreholes with between 2 and 4 samples and 27 boreholes with more than 4 samples (54 boreholes in total). Data Set II includes 203 samples from 29 of the 54 previous boreholes and 1 additional sample from a boreholes not included in Data Set I (HA3289B).

As for the previous objects the boreholes in this group will also be presented in three groups depending on the number of samples that have been taken over the time. Table 6-14 shows the list of the 10 boreholes with 1 sample included in Data Set I. 7 of them were sampled only once and 3 have other samples in Data Set II. From the total of 17 samples, 3 of them have been categorised as Cat. 3, 7 as Cat. 4 and another 7 as Category 5 (those in Data Set II, due to incomplete major ions). Samples in this group were taken between 1998 and 2005 and they are associated with the projects indicated in Table 6-16 and also to the F56 TRUE Block Scale (in the case of some of the Cat. 5 samples).

There are 17 boreholes in the second group (Table 6-15), 4 boreholes with 2 samples, 7 boreholes with 3 samples and 6 boreholes with 4 samples giving a total of 53 samples. From them, 3 samples are Category 1, 4 are Category 2, 20 are Category 3, and 26 samples are Category 4 (the more or less incomplete set of isotopes is the main reason for the lower categories). Apart from these samples, there are another 48 samples taken from some of these boreholes that have been categorised as Category 5 and included in Data Set II mainly because of the incomplete major ions and, in the case of boreholes KA2051A01 and KA3007A01, because they are collected from the returned water during drilling and not from an isolated borehole section.

Samples in this group were taken between 1996 and 2011 and they were associated with different investigations (Table 6-15).

Finally, there are 27 boreholes in the third group (Table 6-16) with more than 4 samples giving a total of 306 samples in Data Set I. From them 18 are Category 1, 126 samples are Category 2, 47 are Category 3 (mainly because of the isotopes and the long sections), and finally, 115 samples of Category 4. They were all sampled between 1996 and 2011 and they were associated with different investigations (Prototype, KBP1001 Brytning av prototypförvaret, TRUE and True Block Scale, RNR, LTDE, F62 LOT and the monitoring program GWCM).

There are 148 samples from these boreholes that have been categorised as Category 5 and are included in Data Set II (see Table 6-1) mainly because of the incomplete major ions and in some cases a high percent of drilling water or a high charge imbalance (in some samples with complete major ions).

**Table 6-14. List of the 16 boreholes included in this group of objects with only one sample taken (or one sample kept in Data Set I). The table includes the information about the ID number of the sample in Data Set I, the ID code of the borehole, the sample number, the section and the elevation of the middle, the sampling data, the project which the sampling was associated with and the defined category.**

| ID DS I | ID code | Sample no. | Secup | Seclow | Elev. (m.a.s.l.) | Date | Project | Category | |
|---|---|---|---|---|---|---|---|---|---|
| 1 | DA1619A02 | 20406 | 0.00 | 94.45 | | 2010/11/30 | GWCM | 4 | |
| 171 | KA2169A01 | 6214 | 0.00 | 3.77 | –290.98 | 2003/10/07 | F83 TRUE-1 | 4 | |
| 172 | KA2169A02 | 6215 | 0.00 | 4.40 | –290.72 | 2003/10/07 | F83 TRUE-1 | 4 | |
| 173 | KA2169A03 | 6213 | 0.00 | 4.52 | –290.77 | 2003/10/07 | F83 TRUE-1 | 4 | |
| 174 | KA2423A01 | 6212 | 0.00 | 5.04 | –322.77 | 2003/10/07 | F83 TRUE-1 | 4 | |
| 175 | KA2423A03 | 6216 | 0.00 | 3.10 | –322.95 | 2003/10/07 | F83 TRUE-1 | 4 | |
| 231 | KA2865A01 | 2917 | 25.33 | 27.73 | –381.46 | 1999/04/27 | Select-2 | 4 | 5 |
| 318 | KA3510A | 6762 | 110.00 | 124.00 | –507.23 | 2005/10/07 | GWCM | 3 | 5(5) |
| 327 | KA3545G | 2478 | 0.00 | 8.04 | –453.05 | 1998/03/02 | F63 PROTOTYPE | 3 | |
| 365 | KA3566G01 | 2886 | 12.20 | 19.80 | –459.83 | 1999/04/09 | GWCM | 3 | 5 |

**Tabla 6-15. List of the 17 boreholes included in this group of objects with 2, 3 and 4 samples for the same section. They are sorted alphabetically by the ID code inside each group. The table includes the information about the ID code of the borehole, the sample number, the section and the elevation of the middle, the project which the sampling was associated with, the sampling date, the defined category (including the number of samples corresponding to Cat. 5, between brackets) and the ID number of the sample in Data Set I.**

| ID code | Sample no. | Elev. (m.a,s.l.) | Secup | Seclow | Project | Start date | Category | | ID DS I |
|---|---|---|---|---|---|---|---|---|---|
| **Boreholes with 2 samples** | | | | | | | | | |
| HMJ01 | 20709 | –33.48 | 37.50 | 46.00 | F4P1 Kemimonit. | | | | |
| | 20932 | | | | | | | | |
| KA2051A01 | 20615 | –324.17 | 78.00 | 89.00 | TUDP002 Utbyggnad Äspö | 2011/02/16 | 4 | 5 | 151 |
| | 20614 | –339.02 | 99.85 | 119.59 | | | 4 | 5(19) | 152 |
| KA3065A02 | 6010 | –409.11 | 7.50 | 13.00 | F79 LTDE | 2003/04/10 | 4 | 5(2) | 245 |
| | 20972 | –409.11 | 7.50 | 13.00 | GWCM | 2011/10/12 | 3 | | 246 |
| KA3386A05 | 6753 | –446.14 | 0.00 | 4.60 | GWCM | 2005/10/06 | 4 | | 313 |
| | 14403 | –446.15 | 0.00 | 4.78 | | 2007/10/01 | 1 | | 314 |
| **Boreholes with 3 samples** | | | | | | | | | |
| KA3007A01 | 20716 | –403.37 | 9.30 | 12.36 | TUDP002 Utbyggnad Äspö | 2011/04/15 | 4 | 5(9) | 239 |
| | 20738 | –404.35 | 12.00 | 17.36 | | 2011/05/05 | 4 | | 240 |
| | 20745 | –456.11 | 222.00 | 227.76 | | 2011/05/18 | 4 | | 241 |
| KA3386A02 | 6748 | –446.30 | 0.00 | 4.60 | GWCM | 2005/10/05 | 4 | | 303 |
| | 14400 | –446.43 | 0.00 | 6.20 | | 2007/10/01 | 2 | | 304 |
| | 14405 | | | | | | 4 | | 305 |
| KA3386A03 | 6747 | –446.28 | 0.00 | 4.60 | GWCM | 2005/10/05 | 4 | | 306 |
| | 14401 | –446.36 | 0.00 | 5.56 | | 2007/10/01 | 2 | | 307 |
| | 14406 | | | | | | 4 | | 308 |
| KA3386A06 | 6755 | –446.14 | 0.00 | 4.60 | GWCM | 2005/10/06 | 4 | | 315 |
| | 14404 | –446.22 | 0.00 | 5.59 | | 2007/10/01 | 2 | | 316 |
| | 14408 | | | | | | 4 | | 317 |
| KA3590G02 | 2889 | –456.57 | 8.30 | 16.30 | GWCM | 1999/04/13 | 3 | | 400 |
| | 2569 | –458.46 | 0.00 | 30.05 | F63 PROTOTYPE | 1998/07/01 | 4 | | 401 |
| | 2563 | –465.71 | 24.00 | 27.00 | | 1998/06/26 | 3 | | 402 |
| KA3593G | 2479 | –462.82 | 0.00 | 30.02 | F63 PROTOTYPE | 1998/03/02 | 3 | | 403 |
| | 2570 | | | | | 1998/07/01 | 4 | | 404 |
| | 2908 | –452.28 | 1.30 | 7.30 | GWCM | 1999/04/15 | 3 | | 405 |
| KXTT5 | 3677 | –392.78 | 9.61 | 9.81 | F83 TRUE-1 | 2001/11/22 | 3 | 5(5) | 818 |
| | 3700 | | | | | 2001/12/10 | 4 | | 819 |
| | 3699 | –395.02 | 10.81 | 25.80 | | 2001/12/11 | 4 | | 820 |
| **Boreholes with 4 samples** | | | | | | | | | |
| KA3386A04 | 6749 | –446.19 | 0.00 | 4.60 | GWCM | 2005/10/05 | 4 | | 309 |
| | 14402 | –446.28 | 0.00 | 5.59 | | 2007/10/01 | 1 | | 310 |
| | 14407 | | | | | 2007/10/01 | 4 | | 311 |
| | 14530 | | | | | 2008/05/26 | 1 | | 312 |
| KA3572G01 | 2928 | –451.78 | 1.30 | 5.30 | F63 PROTOTYPE | 1999/05/17 | 4 | | 372 |
| | 6051 | –452.48 | 2.70 | 5.30 | | 2003/08/11 | 3 | | 373 |
| | 6296 | | | | | 2004/04/02 | 4 | | 374 |
| | 6939 | | | | | 2006/07/12 | 2 | | 375 |
| KF0051A01 | 3039 | –448.88 | 4.66 | 5.26 | F80P1 Matrix | 1999/12/16 | 4 | 5 | 442 |
| | 3680 | –448.88 | 4.66 | 5.26 | | 2001/10/16 | 3 | | 443 |
| | 3679 | –447.84 | 6.26 | 7.85 | | | 3 | 5(2) | 444 |
| | 3678 | –446.77 | 8.85 | 9.55 | | | 4 | 5 | 445 |
| KF0066A01 | 3889 | –454.10 | 0.00 | 60.11 | F80P1 Matrix | 2003/02/13 | 3 | | 446 |
| | 6092 | | | | | 2003/08/29 | 4 | | 447 |
| | 3890 | –455.95 | 0.00 | 70.09 | | 2003/02/13 | 3 | | 448 |
| | 6093 | | | | | 2003/08/29 | 4 | | 449 |
| KJ0050F01 | 2833 | –448.20 | 12.64 | 12.84 | Microbe | 1999/03/19 | 4 | | 545 |
| | 14629 | | | | GWCM | 2008/09/18 | 3 | | 546 |
| | 14436 | –449.67 | 13.84 | 46.79 | GWCM | 2007/10/02 | 3 | | 547 |
| | 14971 | | | | | 2009/09/24 | 3 | | 548 |
| KZ0027A | 2369 | –418.58 | 3.00 | 90.48 | F64 Demoförvar | 1996/12/16 | 3 | 5(8) | 821 |
| | 2374 | | | | | 1997/01/20 | 3 | | 822 |
| | 2378 | | | | | 1997/02/03 | 3 | | 823 |
| | 2380 | | | | | 1997/02/18 | 3 | | 824 |

**Table 6-16. Boreholes, sections (including the elevation, m.a.s.l., of the middle of the section) and samples corresponding to this object type (operation phase) with more than 4 samples. Despite being associated with specific projects or experiments, these boreholes and samples are included in Data Sets I and II. The column with comments indicate some specific information about the samples. Some abbreviations are used in this column in order to shorten the text: Cat for Category, DSI and DSII for Data Sets I and II, CI for charge imbalance, init. cond. for initial conditions and series for sample or time series.**

| Borehole section and vertical elevation (m) | Tot no. | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **HG0038B01**<br>(–446.73) 1–3.6 | 10 | | 7 | 1 | | 1 | 1 | 9 good quality samples in DSI and 1 (Cat. 5) in DSII (incomplete major ions, only anions and isotopes). Samples taken between 1997 and 2011 associated with F62 LOT and GWCM. |
| **KA2563A** | 25 | | | | | | 9 | Several sections (except for the first one, all very short). 16 very good samples in DSI and 9 in DSII (incomplete major ions, only Cl and $HCO_3^-$, some with environmental isotopes and one with no data). Category 4 samples due to the inadequate sample or time series. All the samples were taken between 1999 and 2002 associated with F56 TRUE Block Scale, and GWCM. |
| (–451.78) 146–186 | 1 | | | | | | 9 | |
| (–466.54) 187–190 | 8 | | 6 | 1 | | 1 | | |
| (–478.63) 206–208 | 2 | | | | | 2 | | |
| (–488.38) 220–223 | 1 | | | | | 1 | | |
| (–499.07) 236–241 | 1 | | | | | 1 | | |
| (–502.62) 242–246 | 3 | | 3 | | | | | |
| **KA3065A03** | 20 | | | 1 | | 8 | 11 | Several short sections. 9 low quality samples (incomplete ions and isotopes) in DSI and 11 in DSII (incomplete major ions, most of them only data for sulphide). Samples were taken associated with F79 LTDE between 2000 and 2006. |
| (–408.47) 0–10.4 | 1 | | | | | 1 | 11 | |
| (–408.82) 9–10.2 | 1 | | | | | 1 | | |
| (–408.87) 10.4–10.7 | 3 | | | | | 3 | | |
| (–408.89) 10.7–11.2 | 4 | | | 1 | | 3 | | |
| **KA3539G** | 8 | 2 | 1 | 3 | | 2 | | One section with the whole length of the borehole and another quite short section. All the samples are included in Data Set I. Reasonably good samples except for 3 long sections (Cat. 3) and 2 incomplete isotopes (Cat. 4).<br>They were taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| (–463.96) 0–30 | 3 | | | 2 | | 1 | | |
| (–465.66) 15.8–17.6 | 5 | 2 | 1 | 1 | | 1 | | |
| **KA3542G01** | 11 | 2 | 1 | 1 | | 5 | 2 | Several short sections (except for the first one that covers the whole borehole length). 9 samples in DSI some very good quality samples, and others Cat. 4 due to the incomplete isotopes or the inadequate series. There are two Cat. 2 due to incomplete major ions (only data for Fe). Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| (–459.66) 0–30 | 1 | | | | | 1 | | |
| (–460.70) 15–18 | 1 | | | | | 1 | | |
| (–462.82) 18–21 | 7 | 2 | 1 | 1 | | 2 | 1 | |
| (–464.94) 21–24 | 2 | | | | | 1 | 1 | |
| **KA3542G02**<br>(–451.5/–459.5) 0–30 | 9 | 1 | 1 | 1 | | 5 | 1 | Several irregular but short sections (except the first one over the whole borehole length). 8 samples in DSI and 1 in DSII (incomplete major ions). Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| **KA3548A01**<br>(–446.8/–447.6) 5–21 | 11 | | | | | | 4 | Several irregular but short sections. 7 samples in DSI and 4 in DSII (two due to incomplete major ions and another two due to high charge imbalance). Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret, F56 TRUE Block Scale and GWCM. |
| **KA3554G01**<br>(–464.7/–466.8) 21–27 | 8 | | | | | | 1 | Several irregular but short sections. 7 good samples in DSI and 1 sample in DSII due to a high charge imbalance. Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| **KA3554G02**<br>(–458.3/–459.4) 0–30 | 6 | | 3 | | | 3 | | Several irregular and short sections (except the first one that covers the whole borehole length). Cat. 4 samples due to the inadequate series and incomplete isotopes. Samples taken between 1998 and 2010 associated with F63 Prototype and KBP1001 Brytning av prototypförvaret. |

| Borehole section and vertical elevation (m) | Tot no. | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **KA3566G02**<br>(–460.3/–451.3) 0–30 | 7 | 1 | 2 | | | 3 | 1 | Several irregular and short sections (except the first one that covers the whole borehole length). Cat. 4 samples mainly due to the inadequate series. 6 samples in DSI and 1 sample in DSII (no data). Samples taken between 1998 and 2010 associated with F63 Prototype and KBP1001 Brytning av prototypförvaret. |
| **KA3573A** | 22 | | 11 | 3 | | 4 | 4 | Several sections (some of them quite long). 18 good samples in DSI (only four Cat. 4 samples due to the inadequate series) and 4 in DSII (only data for anions and 2 of them with environmental isotopes). Samples taken between 1998 and 2008 associated with F63 Prototype, F56 TRUE Block Scale and GWCM. |
| (–446.78) 0–40 | 3 | | | | | 2 | 1 | |
| (–446.43) 4.5–17 | 3 | | | | | 2 | 1 | |
| (–447.11) 18–40 | 5 | | | 3 | | | 2 | |
| (–446.87) 21–24 | 5 | | 5 | | | | | |
| (–447.26) 26–40 | 6 | | 6 | | | | | |
| **KA3590G01**<br>(–450.6/–464.1) 1.5–30 | 8 | | 2 | 1 | | 3 | 2 | Several irregular and reasonably short sections. 6 samples in DSI and 2 in DSII (high charge imbalance). Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| **KA3600F** | 46 | | | | | | 10 | Several sections. 36 very good samples in DSI and 10 in DSII (mainly due to incomplete major ions, no data or only anions or only sulphide). Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. Some Cat. 5 samples were also associated with F56 TRUE Block Scale and to F4P1 Kemimonitering. |
| (–445.94) 4.5–21 | 4 | | 3 | | | | 1 | |
| (–446.63) 22–50 | 5 | | | 4 | | | 1 | |
| (–446.78) 40.5–42 | 21 | 5 | 8 | 4 | | 1 | 3 | |
| (–446.94) 43–50.1 | 16 | 1 | 8 | 2 | | | 5 | |
| **KG0021A01**<br>(–441.6/–434.8)<br>10–41 | 15 | 2 | 1 | 1 | | 10 | 1 | Several secions of 1 meter. 14 low quality samples in DSI due to the inadequate sample or time series. One sample in DSII due to incomplete major ions. Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| **KG0048A01**<br>(–433.2/–438.7)<br>0–54.7 | 13 | 1 | 2 | 1 | | 8 | 1 | Several irregular secions of 1 meter. 12 low quality samples in DSI (mainly due to the inadequate series but some sample have incomplete isotopes and even major ions). Only one Category 5 sample in DSII due to a high charge imbalance. Samples taken between 1998 and 2010 associated with F63 Prototype, KBP1001 Brytning av prototypförvaret and GWCM. |
| **KI0023B** | 45 | | | | | | 26 | Several sections (most of them short). 19 good samples in DSI and 26 in DSII (mainly due to incomplete major ions but also high charge imbalance in four samples and high percent of drilling water in another 4).<br>Samples taken between 1997 and 2002 associated with TRUE, F56 TRUE Block Scale and GWCM. |
| (–455.66) 4.6–40.4 | 8 | | | | | 1 | 7 | |
| (–462.58) 41.4–42.4 | 5 | | 2 | | | | 3 | |
| (–467.86) 43.4–69.9 | 4 | | | | | 2 | 2 | |
| (–473.16) 70.9–71.9 | 10 | | 5 | 1 | | | 4 | |
| (–478.20) 84.7–86.2 | 8 | | 4 | 1 | | | 3 | |
| (–487.66) 111.2–112.7 | 6 | | 2 | | | | 4 | |
| (–503.56) 113.7–200.7 | 4 | | | | | 1 | 3 | |
| **KI0025F**<br>(–477.05/ –501.6)<br>86–169.5 | 27 | | 12 | 3 | | | 12 | Several irregular sections. 15 good samples in DSI and 12 in DSII (mainly due to incomplete major ions, but 2 of them have a very high percent of drilling water). Samples taken between 1997 and 2004 associated with TRUE, F56 TRUE Block Scale and GWCM. |
| **KI0025F02**<br>(–467.3/–518.9)<br>38.5–204.2 | 35 | | 12 | | | 7 | 16 | Several irregular sections. 19 good samples in DSI (Cat. 4 samples due to the inadequate series) and 16 in DSII (mainly due to incomplete major ions, but 1 of them have a very high percent of drilling water). Samples taken between 1998 and 2004 associated with TRUE, F56 TRUE Block Scale and GWCM. |

| Borehole section and vertical elevation (m) | Tot no. | Number of samples in each category | | | | | | Comments |
|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 3b | 4 | 5 | |
| **KI0025F03**<br>(–476.1/–512.2)<br>55–134 | 14 | | | | | 9 | 5 | Several irregular sections (all quite short). 9 low quality samples in DSI (inadequate series) and 5 in DSII (mainly due to incomplete major ions, but 2 of them have a very high percent of drilling water). Samples taken between 2000 and 2005 associated with TRUE, F56 TRUE Block Scale and GWCM. |
| **KJ0044F01**<br>(–447.76) 1–17.3 | 9 | | 5 | 1 | | 1 | 2 | 7 good samples in DSI and 2 in DSII (incomplete major ions and high charge imbalance). Samples taken between 1999 and 2009 associated with F58 RNR and then to GWCM. |
| **KJ0052F01** | 6 | | 4 | 1 | | 2 | | Three sections (short except for the first one). Reasonably good samples in DSI. Samples taken between 2007 and 2011 associated with GWCM. |
| (–448.84) 3.2–42.7 | 1 | | | | | 1 | | |
| (–450.52) 43.7–43.9 | 1 | | 1 | | | | | |
| (–450.81) 44.9–50.1 | 4 | | 3 | 1 | | | | |
| **KJ0052F02** | 12 | | | | | | 2 | 2 sections. 10 quite good samples in DSI (except for some long sections) and 2 in DSII (incomplete major ions).<br>Samples taken between 1999 and 2011 associated with F58 RNR and then to GWCM. |
| (–447.35) 0–21.4 | 11 | | | 8 | | 1 | 2 | |
| (–447.66) 15–21.4 | 1 | | 1 | | | | | |
| **KJ0052F03** | 5 | | 2 | 1 | | 2 | | 3 short sections (the first one covering the whole borehole length). Samples taken between 1999 and 2009 associated with F58 RNR and then to GWCM. |
| (–447.31) 0–10.6 | 1 | | | | | 1 | | |
| (–447.57) 8.1–10.1 | 1 | | | | | 1 | | |
| (–447.66) 10.4–10.6 | 3 | | 2 | 1 | | | | |
| **KXTT1** | 15 | | 2 | | | 4 | 9 | Several short sections. 6 poor quality samples in DSI (incomplete isotopes and inadequate monitoring) and 9 in DSII (incomplete major ions, three of them without data, the others only Cl and bicarbonate and some also environmental isotopes). Samples taken between 1995 and 2001 associated with F83 TRUE-1. |
| (–398.88) 8.5–10.5 | 4 | | | | | 1 | 3 | |
| (–403.17) 15–16 | 8 | | 2 | | | 2 | 4 | |
| (–408.45) 17–28.8 | 3 | | | | | 1 | 2 | |
| **KXTT2** | 15 | | 2 | | | 6 | 7 | Several short sections. 8 samples in DSI and 7 in DSII (incomplete major ions, only Cl and bicarbonate and some of them with environmental isotopes). Samples taken between 1995 and 2001 associated with F83 TRUE-1. |
| (–395.76) 3–6.5 | 8 | | | | | 1 | 7 | |
| (–401.19) 11.5–13.5 | 2 | | | | | 2 | | |
| (–402.94) 14.5–15.5 | 4 | | 2 | | | 2 | | |
| (–404.60) 16.5–18.3 | 1 | | | | | 1 | | |
| **KXTT3** | 30 | | 9 | 4 | | 7 | 10 | Several short sections. 20 good samples in DSI and 10 in DSII (incomplete major ions, one of the samples without data, the others only Cl and bicarbonate and some also environmental isotopes). Samples taken between 1995 and 2001 associated with F83 TRUE-1 and GWCM. |
| (–394.38) 3.2–7.9 | 3 | | | | | 1 | 2 | |
| (–396.70) 8.9–9.9 | 4 | | 1 | 1 | | 1 | 1 | |
| (–398.65) 10.9–14.4 | 20 | | 8 | 3 | | 4 | 5 | |
| (–400.90) 15.4–17.4 | 3 | | | | | 1 | 2 | |
| **KXTT4** | 21 | | | | | | 10 | Several short sections. 11 poor quality samples in DSI and 10 in DSII (incomplete major ions, three of the samples without data, the others only Cl and bicarbonate and some also environmental isotopes). Samples taken between 1995 and 2001 associated with F83 TRUE-1 and GWCM. |
| (–396.81) 8.4–10.9 | 6 | | 2 | | | 1 | 3 | |
| (–398.59) 11.4–13.9 | 7 | | 1 | 1 | | 2 | 3 | |
| (–399.03) 12.9–13.9 | 2 | | | | | 2 | | |
| (–402.45) 14.9–23.4 | 6 | | | | | 2 | 4 | |

### 6.4.3 Boreholes, borehole sections and samples in Data Set IV (Group B)

This section presents those boreholes drilled after the construction of the tunnel for specific projects and experiments that disturbed the groundwaters sampled and therefore they were discarded from the original set of water samples since the beginning as they were considered unsuitable for modelling purposes. They were stored in Data Set IV.

Some of the samples in this data set correspond to boreholes only included in this group (Table 6-17). However, there are other samples that were taken from boreholes used for other projects and some of their samples are in Data Sets I or II. Table 6-18 lists these boreholes indicating the project and number of samples taken included in this Data Set IV, and the rest of the projects in which samples from the same boreholes were taken and are included in Data Sets I and II.

There are 76 boreholes in Data Set IV and a total of 482 samples. 48 boreholes are only in this data set and 28 have samples in Data Set I and II. In all the cases, the samples included in this data set are considered unsuitable for modelling. However, as they are associated with very specific experiments, they could be very useful for comparison with similar experiments in the future.

**Table 6-17. List of the 48 boreholes only included in Data Set IV. The list is sorted alphabetically by the name of the project (not the borehole). The number of samples taken in each borehole is indicated between brackets besides the ID code for the borehole.**

| Borehole (No. of samples) | Project | Borehole (No. of samples) | Project |
|---|---|---|---|
| KA2198A (6) | ÄFS – svavel och multielement<br>F82 Microb, F82P1 MICOMIG | | |
| KR0014G01 (1) | Concrete & Clay | KI0010B01 (5) | SU32516 Fintätning |
| KA2368A01 (1) | Crock | KI0016B01 (2) | SU32516 Fintätning |
| KA2370A01 (1) | Crock | KI0014B01 (3) | SU32516 Fintätning |
| DA3147G01 (1) | F122 LASGIT | MS0010G01 (4) | SU32516 Fintätning |
| KQ0036G01 (1) | F125 Alternative Buffer Material | MS0050G01 (4) | SU32516 Fintätning |
| KQ0040G01 (1) | F125 Alternative Buffer Material | SS0004G01 (1) | SU32516 Fintätning |
| KF0069A01 (11) | F50 FUD Allmänt | SS0004G21 (1) | SU32516 Fintätning |
| KXBLOTA1 (2) | F62 LOT | SS0004H03 (1) | SU32516 Fintätning |
| KXBLOTS1 (2) | F62 LOT | SS0004I03 (1) | SU32516 Fintätning |
| PXP0KFA01 (3) | F63 PROTOTYPE | SS0020A12 (1) | SU32516 Fintätning |
| PXP0KFA04 (2) | F63 PROTOTYPE | SS0020A22 (1) | SU32516 Fintätning |
| PXPKBU101 (2) | F63 PROTOTYPE | SS0020B14 (1) | SU32516 Fintätning |
| PXPKBU102 (2) | F63 PROTOTYPE | SS0020B16 (1) | SU32516 Fintätning |
| PXPKBU106 (1) | F63 PROTOTYPE | SS0020D03 (1) | SU32516 Fintätning |
| PXPKBU108 (2) | F63 PROTOTYPE | SS0020I14 (1) | SU32516 Fintätning |
| KXZC2 (2) | F66 ZEDEX | SS0029G03 (1) | SU32516 Fintätning |
| KXZC7 (1) | F66 ZEDEX | SS0032A02 (1) | SU32516 Fintätning |
| KA3386A01 (3) | F82 Microb | SS0032F01 (1) | SU32516 Fintätning |
| HA1127B (1) | F82 Microb | SS0040A01 (5) | SU32516 Fintätning |
| KA1362A01 (3) | F82P1 MICOMIG | SS0045B01 (1) | SU32516 Fintätning |
| SA1759A (1) | F91 COLLOID | SS0045B02 (1) | SU32516 Fintätning |
| DA1619A02 (5) | KBS3-H | SS0048G10 (1) | SU32516 Fintätning |
| DA1622A01 (1) | KBS3-H | TASS (8) | SU32516 Fintätning |
| KA2599G01 (1) | Rock mechanical measurements | | |

**Table 6-18. List of the 28 boreholes included in Data Set IV that have other samples suitable for modelling associated with other projects or experiments (indicated in the right column) and, therefore, they have already been included in the previous objects.**

| ID code | No samp | Project in Data Set IV | Other Projects in other data sets |
|---|---|---|---|
| **Surface** | | | |
| KAS03 | 1 | PRAS1001 | GWCM |
| Probing | | | |
| SA1327B | 5 | F50 FUD Allmänt | 750–3,191 m |
| SA1730A | 1 | F61 Backfill&Plug | 750–3,191 m, GWCM, F4P1 Kemimonitering |
| SA2880A | 1 | F61 Backfill&Plug | GWCM, F4P1 Kemimonitering |
| | 1 | F83 TRUE-1 | |
| **Others (construction phase)** | | | |
| HA1327B | 1 | ÄFS – svavel och multielement | 750–3,191 m |
| | 12 | F50 FUD Allmänt | ÄFS – svavel och multielement TotDiss |
| HD0025A | 1 | F61 Backfill&Plug | GWCM, F4P1 Kemimonitering, F63 PROTOTYPE, Select, F61 Backfill&Plug |
| KA1061A | 1 | ÄFS – svavel och multielement | 750–3,191 m, GWCM, F4P1 Kemimonitering |
| KA1755A | 1 | F61 Backfill&Plug | GWCM, 750–3,191 m, F91 COLLOID |
| KA2162B | 17 | F50 FUD Allmänt | 750–3,191 m, GWCM, F4P1 Kemimonitering |
| KA2598A | 1 | F125 Alternative Buffer Material | GWCM, 750–3,191 m |
| | 1 | F58 RNR | |
| KA2858A | 5 | TSF137 SWIW-test syntetiskt grundvatten | GWCM, Select |
| KA2862A | 1 | F57 REX | GWCM |
| | 2 | Select | F61 Backfill&Plug |
| KA3010A | 1 | ÄFS – svavel och multielement | GWCM, Select |
| KA3110A | 4 | F82P1 MICOMIG | GWCM, Select |
| | 13 | F82P2 MICORED | |
| | 2 | GWCM | |
| | 4 | KBP4001 | |
| | 1 | ÄFS – svavel och multielement | |
| KA3385A | 4 | KBP4001 | F58 RNR, F91 COLLOID, GWCM, F56 TRUE Block Scale |
| KR0013B | 1 | ÄFS – svavel och multielement | GWCM, REDOX |
| KR0015B | 1 | ÄFS – svavel och multielement | GWCM, REDOX |
| **Projects (operation phase)** | | | |
| KA3386A02 | 23 | F77P3 Mini Can | |
| KA3386A03 | 24 | F77P3 MINI-CAN | |
| KA3386A04 | 24 | F77P3 MINI-CAN | |
| KA3386A05 | 18 | F77P3 MINI-CAN | |
| KA3386A06 | 23 | F77P3 MINI-CAN | |
| KA3542G01 | 1 | PRAS1001 | F63 PROTOTYPE |
| KA3600F | 1 | Crock | F63 PROTOTYPE |
| KG0048A01 | 1 | F63 PROTOTYPE | F63 PROTOTYPE |
| KJ0050F01 | 51 | F82 Microb | |
| | 1 | F82P1 MICOMIG | |
| | 1 | F82P2 MICORED | |
| | 1 | ÄFS – svavel och multielement | |
| KJ0052F01 | 49 | F82 Microb | |
| | 1 | F82P1 MICOMIG | |
| | 6 | F82P2 MICORED | |
| | 1 | ÄFS – svavel och multielement | |
| | 1 | F58 RNR | |
| KJ0052F03 | 49 | F82 Microb | F58 RNR |
| | 1 | F82P1 MICOMIG | |
| | 1 | F82P2 MICORED | |
| | 1 | ÄFS – svavel och multielement | |

## 6.5 Weirs (Mätvallar)

### 6.5.1 Description

The water inflow along the tunnel is collected in a series of water dams and weirs, see Figures 6-2 and 6-3. Drain pipes from each dam lead the water to a gauging box equipped with a v-notch weir (Thomson weir) for water level and flow measurements. Four special pump sumps finally collect the drainage water which is pumped to the surface (Almén and Stenberg 2005). The list of weirs is shown in Table 6-19. Although the main objective of the weir system is to monitor the water inflow along the different sections of the tunnel, electric conductivity and Cl concentration were also measured almost yearly in order to monitor the evolution of the water salinity with time.

**Table 6-19. List of the weirs located along the tunnel.**

| | | | | | |
|---|---|---|---|---|---|
| MA0682G | MA2699G | MA2028G | MA2699G | MA3411G | MS0010G01 |
| MA1033G | MA1584G | MA2178G | MA2840G | MA3426G | MS0033G01 |
| MA1033G | MA1659G | MA2357G | MA2994G | MA3591 | MS0050G01 |
| MA1232G | MA1745G | MA2496G | MA3179G | MF0061G | |
| MA1372G | MA1883G | MA2587G | MA3384G | MG0004G | |

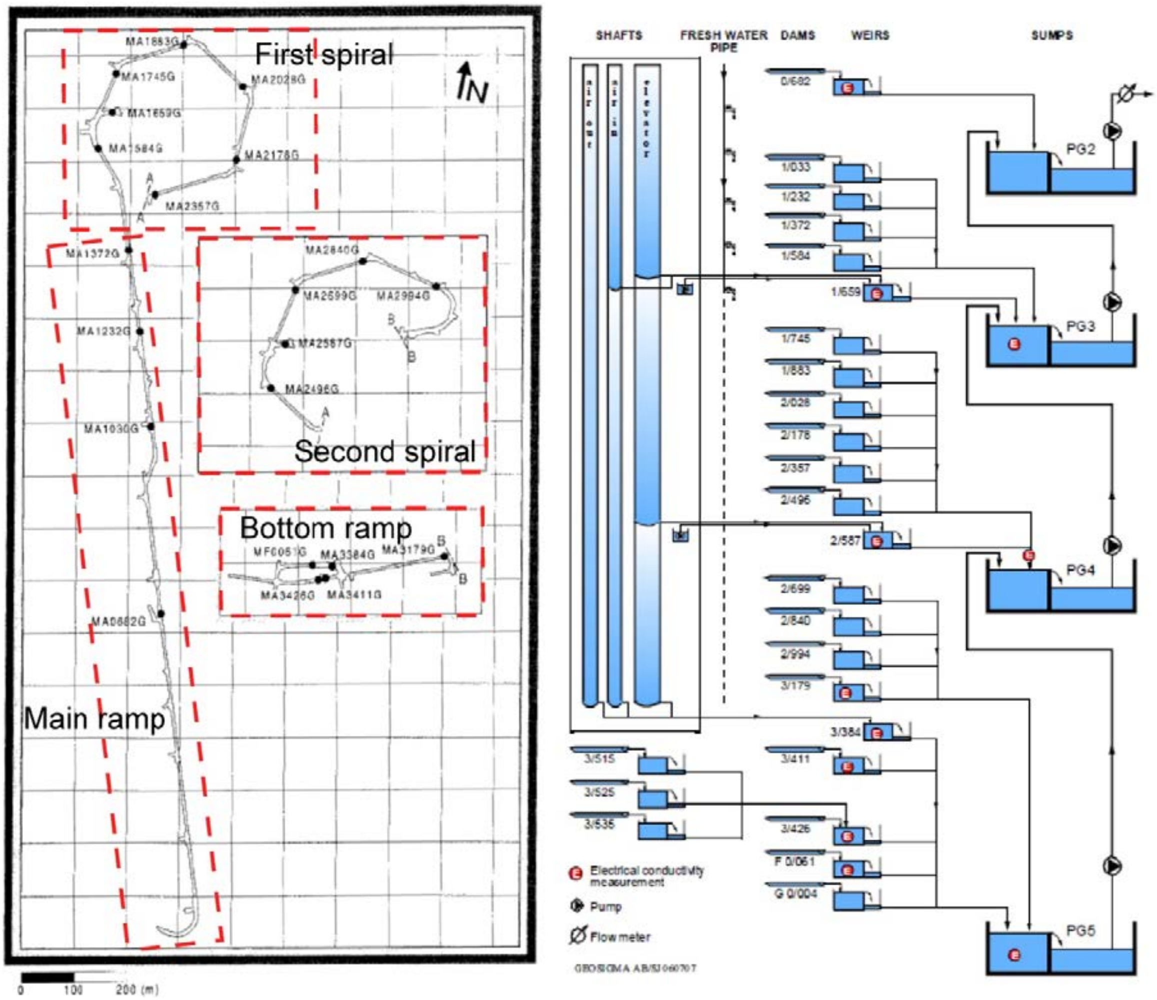

*Figure 6-2. Left: plan of the weirs along the tunnel (modified from Rhén et al. 1997c). Right: schematic picture showing the tunnel drainage system (taken from Berlin and Hardenby 2008).*

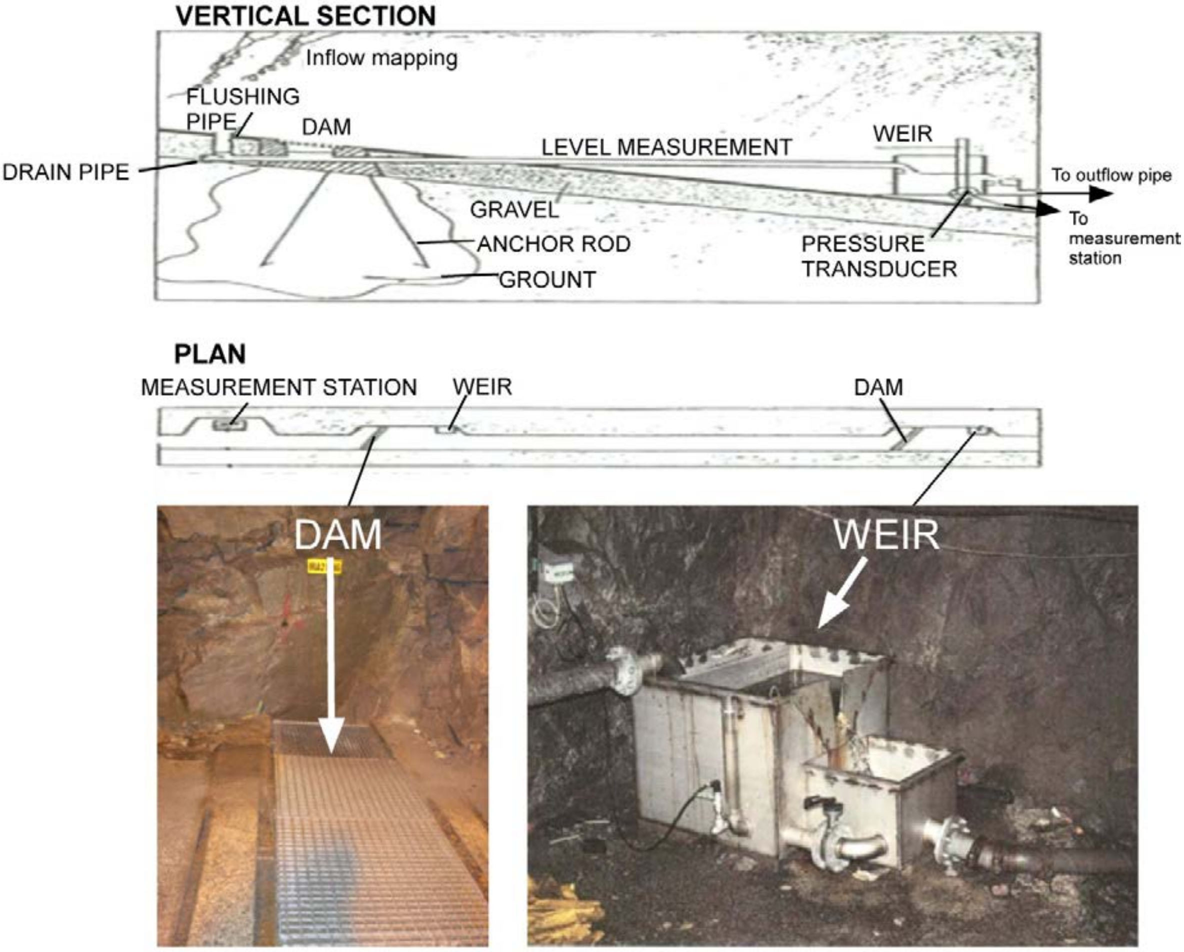

***Figure 6-3.*** *Flow measurements from dam and weir. The total flow into and out from the tunnel were measured as well as flow into a number of tunnel sections. Approximately every 150 m along the tunnel a concrete dam was built in the tunnel floor and the dam was connected by pipework to a weir downstream. In this way the flow into a number of tunnel sections could be measured continuously. The Measurement Station (MS) is a part of The Hydro Monitoring System (HMS). Normally the level is monitored every 10th second but stored only every 30th minute, unless the change since the last stored value exceeds a predefined change of value, normally 1 mm. (Modified from Rhén et al. 1997b. Top: basic layout of the flow measurement. Bottom: Dam and weir in the Äspö HRL.)*

### 6.5.2 Weirs and samples

There are 439 samples taken in these special points but unfortunately the number of parameters analysed are very scarce and heterogeneously distributed, thus limiting their use. The only parameter that was always analysed in the laboratory was the electrical conductivity, so, this is the only value that can be traced over the space and time. There are only 346 samples with the chloride content (in most of them only chloride was analysed) and only 41 of them contain complete data for major and minor elements. Only 13 samples show a complete set of analyses corresponding to the more recent project SU32516 Fintätning; 6 of them contain environmental isotope information.

In general, all the sampling points (weirs) have been sampled at the same time, although there are some exceptions that will be described below and are detailed in Table 6-20. Except for samples taken during 1993 and 1995, which are considered part of the project 750–3,191, the rest of the samples were taken during the monitoring programme GWCM.

The sampling commenced in 1993 when the construction of the tunnel had almost finished and at this juncture weirs were present down to 2,028 m along the tunnel. During the summer of 1993 2 or 3 samples were taken in each weir and there are values for the sampling flow, the pH and EC in lab, and the chloride content.

There are no samples taken in 1994. In 1995, all the weirs were sampled (down to the final ramp). In most of the cases 4 to 5 samples were taken but there are data for major and minor elements only in two of them; the rest of the samples only have the conductivity value. No samples were taken during the following two years (1996 and 1997).

During 1998 to 2001 samples were taken from all the weirs, twice in spring and autumn during the first two years, or once a year in autumn, during 2000 and 2001. These contain data for the sampling flow, the chloride content and the electrical conductivity and pH measured in the laboratory. The period between 2002 and 2007 was covered with one sample per year in each weir where chloride, electrical conductivity and pH were analysed. There are two exceptional cases during 2007: 1) weir MA1659 was sampled in the framework of two different projects (apart from the usual monitoring); 1 sample from F49 Hydrogeologi ämnesansvar and 2 from the BACLO Large Scale Test were analysed for major and minor elements; 2) weir MA3426 which was analysed within the framework of the HRL O&M project; the sample contains a complete chemical characterisation (except for Cl).

Sampling campaigns during 2008, 2009 and 2010 are more heterogeneous although in general all the weirs follow the same sampling routine, i.e. one sample for each weir and each year. The data available for the samples taken in 2008 are drilling water, Uranine, pH and electrical conductivity measured in the laboratory; in 2009 there are data for pH and electrical conductivity, density and chloride content; in 2010 the same approach as in 2009 was conducted with field measurements for pH, conductivity and temperature.

The special cases for these latest years are the following: a) 2008: one of the samples taken in MA3426 has a complete chemical characterisation (including isotopes). Samples taken in MF0061G, MF0004G and MS0010G01 contain data for major and minor elements (and the last one even isotopes). b) 2009: All the samples taken in the weirs in the S-side tunnel (MS0010G01, MS0033G01 and MS0050G01) during this year contain data for drilling water, Uranine, major, minor and some trace elements and 4 of them have isotopes.

**Table 6-20. Number of samples and data analysed for every weir sampling point over the years (Data Set III).**

| Identification code (m. along the tunnel) | Tot no. | Project | Drill wat | Uranine | SFlow | pHl | pHf | Ecl | Ecf | Temp | Dens | Cl | Major | Minor | Isot | Comp | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MA0682G | 21 | MA0682G (0–682 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | 0–750 | | | | x | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000 | 1 | | | | x | x | | x | | | | x | | | | | |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA1033G | 27 | MA1033G (692–1,033 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 9 | | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |

| Identification code (m. along the tunnel) | Tot no. | Project | Drill wat | Uranine | SFlow | pHl | pHf | Ecl | Ecf | Temp | Dens | Cl | Major | Minor | Isot | Comp | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MA1232G | 22 | MA1232G (1,033–1,232 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998 | 2 | GWCM | | | x | x | | x | | | | x | | | | | |
| 1999 | 2 | | | | 1 | x | | x | | | | x | | | | | |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA1372G | 21 | MA1372G (1,232–1,372 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2001 | 1 | | | | x | x | | x | | | | x | | | | | |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA1584G | 22 | MA1584G (1,372–1,584 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA1659G | 17 | MA1659G (1,584–1,659 m) | | | | | | | | | | | | | | | |
| 1998 | 1 | GWCM | | | x | x | | x | | | | x | | | | | |
| 1999 | 2 | | | | x | x | | x | | | | x | | | | | |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2006 | 5 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2007 | 4 | Several projects | | | | x | | x | | | | x | 3 | 3 | | | GWCM, F49 Hydrogeol ämnes, BACLO LScaleT |
| 2008 | 1 | GWCM | x | x | | x | | x | | | | x | | | | | Bicarbonate value included |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA1745G | 21 | MA1745G (1,584–1,745 m) | | | | | | | | | | | | | | | |
| 1993 | 2 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |

| Identification code (m. along the tunnel) | Tot no. | Project | Drill wat | Uranine | SFlow | pHl | pHf | Ecl | Ecf | Temp | Dens | Cl | Major | Minor | Isot | Comp | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MA1883G | 21 | MA1883G (1,745–1,883 m) | | | | | | | | | | | | | | | |
| 1993 | 2 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | | | | 2 | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2028G | 22 | MA2028G (1,883–2,028 m) | | | | | | | | | | | | | | | |
| 1993 | 3 | 750–3,191 | | | x | x | | x | | | | x | | | | | |
| 1995 | 4 | | | | | 2 | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2178G | 19 | MA2178G (2,028–2,178 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2357G | 19 | MA2357G (2,178–2,357 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | 2 | | | 3 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2496G | 19 | MA2496G (2,357–2,496 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | 1 | | | 2 | | x | | | | 1 | 1 | 1 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |

| Identification code (m. along the tunnel) | Tot no. | Project | Drill wat | Uranine | SFlow | pHl | pHf | Ecl | Ecf | Temp | Dens | Cl | Major | Minor | Isot | Comp | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MA2587G | 15 | MA2587G (2,496–2,587 m) | | | | | | | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | X | | | | | HCO$^3$ value also included |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2699G | 19 | MA2699G (2,587–2,699 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | 2 | | | 2 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2840G | 19 | MA2840G (2,699–2,840 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | 2 | | | 2 | | x | | | | 2 | 2 | 2 | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA2994G | 16 | MA2994G (2,840–2,994 m) | | | | | | | | | | | | | | | |
| 1995 | 4 | 750–3,191 | | | | 2 | | x | | | | | | | | | |
| 1999–2001 | 3 | GWCM | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA3179G | 15 | MA3179G (2,840–3,179 m) | | | | | | | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA3384G | 20 | MA3384G (3,179–3,384 m) | | | | | | | | | | | | | | | |
| 1995 | 5 | 750–3,191 | | | | | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |

| Identification code (m. along the tunnel) | Tot no. | Project | Drill wat | Uranine | SFlow | pHl | pHf | Ecl | Ecf | Temp | Dens | Cl | Major | Minor | Isot | Comp | Comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| MA3411G | 20 | MA3411G (3,384–3,411 m) | | | | | | | | | | | | | | | |
| 1995 | 5 | 750–3,191 | | | | | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2008 | 1 | | x | x | | x | | x | | | | | | | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA3426G | 22 | MA3426G (3,411–3,426 m) | | | | | | | | | | | | | | | |
| 1995 | 5 | 750–3,191 | | | | | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2006 | 5 | | | | | x | | x | | | | X | | | | | One sample every year |
| 2007 | 2 | HRL O&M | | | | x | | x | | | | 1 | 1 | 1 | | | Even trance elements (but not Cl) |
| 2008 | 2 | GWCM | x | x | | x | | x | | | | x | x | x | 1 | 1 | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MA3591 | 1 | PROTO-TYPE | x | | | x | | x | | | | | | | | | September 2001 |
| MF0061G | 20 | MF0061G | | | | | | | | | | | | | | | |
| 1995 | 5 | 750–3,191 | | | | | | x | | | | | | | | | |
| 1998–1999 | 4 | GWCM | | | x | x | | x | | | | x | | | | | Two samples every year |
| 2000–2001 | 2 | | | | x | x | | x | | | | x | | | | | One sample every year |
| 2002–2007 | 6 | | | | | x | | x | | | | x | | | | | One sample every year |
| 2008 | 2 | | x | x | | x | | x | | | | x | x | x | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MG0004G | 8 | MG0004G | | | | | | | | | | | | | | | |
| 2002–2007 | 5 | GWCM | | | | x | | x | | | | x | | | | | One sample every year except for 2005 |
| 2008 | 2 | | x | x | | x | | x | | | | x | x | x | | | |
| 2009 | 1 | | | | | x | | x | | | x | x | | | | | |
| 2010 | 1 | | | | | x | x | x | x | x | x | x | | | | | |
| MS0010G01 | 6 | MS0010G01 | | | | | | | | | | | | | | | |
| 2008 | 1 | SU32516 Fintätning | x | x | | x | | x | | | | x | x | x | x | | Even trace elements |
| 2009 | 5 | | 3 | 3 | | x | | x | | | | x | x | X | 2 | X | |
| MS0033G01 | 3 | | x | x | | x | | x | | | | x | x | x | | | Sampled in 2009 even trace elements |
| MS0050G01 | 4 | | 2 | 2 | | x | | x | | | | x | x | x | 2 | 2 | Sampled in 2009 |

# 7 Final Hydrochemical data set

A description and evaluation of the hydrochemical data from the Äspö local area has been presented in the previous chapters. The main objective of this work has been to facilitate future interpretation and modelling work by organising a set of well structured data tables with selected and quality categorised data. This chapter focuses on the description of these tables, their contents and structure.

Apart from the evaluation of the quality of the data, this compilation work had to deal with data stored over a long period of time and some inconsistencies and errors were found in the data content in Sicada (the data base used at present). The corrections and modifications done in the Sicada database are listed in Appendix 2.

Finally, a general view of the main chemical contents in the groundwater samples is presented in the form of plots showing their distribution with depth and chloride content.

## 7.1 Compiled data table for interpretation and modelling

### 7.1.1 Final excel file structure

The whole set of data contains 3,180 groundwater samples collected and analysed during the time period between 1986 and 2011. All of them have been stored in an excel file separated in different data sets according to their suitability for general modelling purposes. This excel file is stored in the SKB documentation system SKBdoc for traceability (SKBdoc 1393008).

- Data Set I: contains 1,585 samples corresponding to Categories 1 to 4.
- Data Set II: contains 674 samples that have been categorised as Category 5 due to incomplete chemical analyses, impact from grouting, high charge imbalance (indicating poor analytical performance), and high percentage of drilling water, etc.
- Data Set III: contains data from the weirs (439 samples).
- Data Set IV: contains 482 groundwater samples from different projects and experiments that have been excluded from modelling purposes as they may have been affected by the experimental conditions, or they may represent sampling conditions not comparable with the regular sampling prototcols (e.g. sampling from a circulating system connected to the sampled borehole section or from a borehole where water has been injected).
- Finally, there are an additional three tables included in the excel file containing additional information that may be used for special purposes, although they are not suitable for regular modelling work. These tables contain the data corresponding to microbes, gasses and matrix porewaters, respectively.

There are two initial sheets in the Excel file with a brief explanation of the dataset contents and a description of the columns included in the datasets. The general structure of the four first dataset tables (Data Set I, II, II and IV) is the same. The columns present thorough information for each sample, from their identification codes, location, date, project which they are associated with, additional information about the purpose of the sampling, the investigation phase or stage, the type of sampling, drilling water, the field and laboratory physicochemical measurements (pH, Eh, T, conductivity) and the all chemical analyses (major, minor, trace elements, isotopes, microbes and gasses if available). The categorisation criteria grades and the final category of the sample, together with some additional columns containing some parameters calculated with PHREEQC, are also included in Data Set I.

Tables with additional information on microbes and gasses only contain columns with specific information about these data apart from their identification information. In both cases, the corresponding sample number of the chemically characterised groundwater sample (when available), is also indicated together with the dataset in which this sample can be found; if there is not a corresponding sample, the closest in time (days) taken in the same section, is indicated in the column "closest SNO". The following columns show the sampling date, the project, the section sampled in the borehole and the corresponding elevation. The rest of the columns report the microbiological or the gas contents, respectively, i.e. total number of cultivated bacteria, ATP, SRB, NRB, IRB and MRB, AA, HA, AM and HM, MOB and CHAB in the microbes table, and the He, Ar, $N_2$, $CO_2$, $O_2$, $CH_4$, $H_2$, CO, $C_2H_2$, $C_2H_4$, $C_2H_6$, $C_3H_8$, $C_3H_6$ and Gas Volume in the gas table.

Matrix porewater table has a completely different structure as it only contains 13 porewater samples. The main difference is that the samples are in columns but the information contained and reported for each sample is basically the same as in the other tables: information about the sample codes, borehole, sections, dates, indication of the laboratory where the samples have been analysed, and the physico-chemical parameters and the chemical and isotopic information.

### 7.1.2 Inconsistencies and errors in the data delivery

The Äspö data have been obtained during a long time period and databases, database structure, sampling and analytical methods have changed and improved with time. In addition, the personnel responsible for data reporting to the database (Sicada or the previous ones) and the quality check procedure have also changed. This has had implications on the stored Äspö HRL data and some of the discovered inconsistencies and errors are indicated below:

- Carbon-14 data from the pre-investigation phase and the first years of tunnel construction were reported as C-14 age and C-14 age corrected for C-13 content. Despite the decision to continue using pmC (percent of modern Carbon), this older reporting system has been used sporadically to this day in parallel with reporting the values as pmC. The problem is that the column labelled "C-14 AGE CORR" contains a mixture of two different types of values, 1) C-14 age corrected for C-13 content, as intended, and 2) the error or standard deviation in the C-14 age determination. In order to avoid any possible future confusion in the final Äspö datasets, when pmC values were missed but C-14 age values were available, these values have been converted to pmC, and the columns C-14 AGE and C-14 AGE CORR have been removed.
- The dissolved gas analyses include dissolved oxygen, however, in reality this is a contamination caused by introduction of air during the sample handling or gas extraction procedure. The reporting of analytical results for dissolved oxygen to the Sicada database has varied with time and three different strategies have been used: 1) The $O_2$ concentration is recorded together with the other gas analyses in Sicada, 2) the $O_2$ concentration is removed as well as the corresponding $N_2$, $CO_2$ and argon concentrations calculated from the $O_2$ concentration in air, and 3) both records are given for the sample, i.e. including the intruded air as well as excluding the air corresponding to the $O_2$ concentration. It is recommended to give both records.
- Information on groundwater flow rate is very often missing. There are two columns for groundwater flow rate in the data delivery table, Q_F (l/min) and SMPL_FLOW (l/min). It is recommended that one of the columns should be used for the considered corrrect flow rate and the other for the sampling flow rate that may be reduced by a valve. For the moment it is unclear which flow has been reported in the few cases where it has been registered in Sicada. It is recommended to report both groundwater flow rates and to be very clear on whether the flow rate is reduced or not. For the moment, these two columns have been removed from the final data sets.
- The most common error found from the data evaluation in the Äspö HRL is in the recorded section limits (Secup and Seclow) in boreholes in the Äspö HRL. However, errors could be avoided by giving the borehole section numbers when storing a sampling activity. The valid section limits will then appear automatically for each sampling activity. The corrections made in the Äspö data sets are indicated in Appendix 2.

There are a very few other occasional inconsistencies and errors and in general they have little or no implications on future modelling work but rather affect the trustworthiness of the Sicada database.

## 7.2 Data selected for modelling

### *Samples representative of the initial conditions*

Data considered representative of the initial conditions, i.e. not disturbed by the tunnel construction, are essential to understand the modifications that have influenced the groundwater system over the years. Many of them relate to surface boreholes sampled during the pre-investigation phase, between 1987 and 1990. The rest correspond to the probing boreholes located just at the front of the tunnel while it was being drilled and, therefore, they were taken during the construction phase (from 1990 to 1995). There are also another small number of samples collected before 1992 from other tunnel boreholes: these probing boreholes have been included to enlarge the initial conditions group because they reasonably represent early conditions.

The surface borehole samples are usually represented by a good time series but they do not have a complete set of environmental isotopes; a detailed description of these samples can be found in Section 6.1.2. The probing boreholes do not have long time or sample series and some of them do not even have a complete set of environmental isotopes (see Section 6.2.2), and this is the reason why most of these samples have been considered as Category 3b, despite having very good grades for the rest of the categorisation criteria (see Section 4.4).

These samples, together with samples taken in the regional area (Laxemar and Simpevarp, see Section 7.2.1.7), represent the general pristine conditions in the hydrogeochemical system.

### *Samples with long sample series*

Samples taken in the same borehole sections over the years (long sample series) are very useful to understand the evolution of the system. They might show changes in chemistry due to disturbances during tunnel construction (Figure 7-1; Left), or they might show a more or less consistent behaviour indicative of a more isolated part of the hydrochemical system barely disturbed by the external activities (Figure 7-1; Right). This kind of analysis can be easily achieved as Data Set I is organised by the amount of samples taken in the boreholes, and therefore, those boreholes with long time and sample series are clearly separated in the excel file. Moreover, the samples in each borehole are sorted by section and date and therefore, evolution plots with time are straightforward (Figure 7-1).

The evolution of the system after the construction of the tunnel also depends on the hydrogeological properties of the fractures (e.g. permeability or interconnection between fractures). These fracture properties affect the period of time needed to reach a new steady state. For instance, Figure 7-1 illustrates that a new stable Cl concentration can be rapidly reached in certain boreholes (e.g. borehole SA1420A), while Cl continues to change over the 10 year period of monitoring in other boreholes (e.g. borehole KA1730A). As most of the changes occurred during the tunnel construction, it is thus strongly recommended to take into consideration the composition of the initial groundwater when working with the evolution of the system from a hydrochemical viewpoint. Without such information, the stability of Cl observed in certain sample series monitored later (e.g. Borehole KA3573A) only provides an indication of a temporary hydrochemical steady state which does not necessarily mean that this stability occurred during tunnel construction (Mathurin et al. 2012).

### *Samples with long time series*

From the SDM experiences in Laxemar and Forsmark (including the SFR extension project) (Smellie et al. 2008, Smellie and Tullborg 2009, Nilsson et al. 2011), samples taken in the same borehole section over a short period of time (time series) have proved to be very useful to give an idea of when the water sample is stabilised and represents the groundwater in the isolated fracture (formation water). They have been used during the categorisation process and during the explorative analyses.

In general, in the process of performing a time series the category of the sample is only chosen when the sample is considered stabilised and representative, and then it undergoes a complete chemical characterisation. The result is that in the earlier part of the time series most of the samples are allocated a low Category 4 (sometimes even 5) but in most of the cases this is only because of the lack of data.

An example of one of this time series in one of the surface boreholes is shown in Figure 7-2.

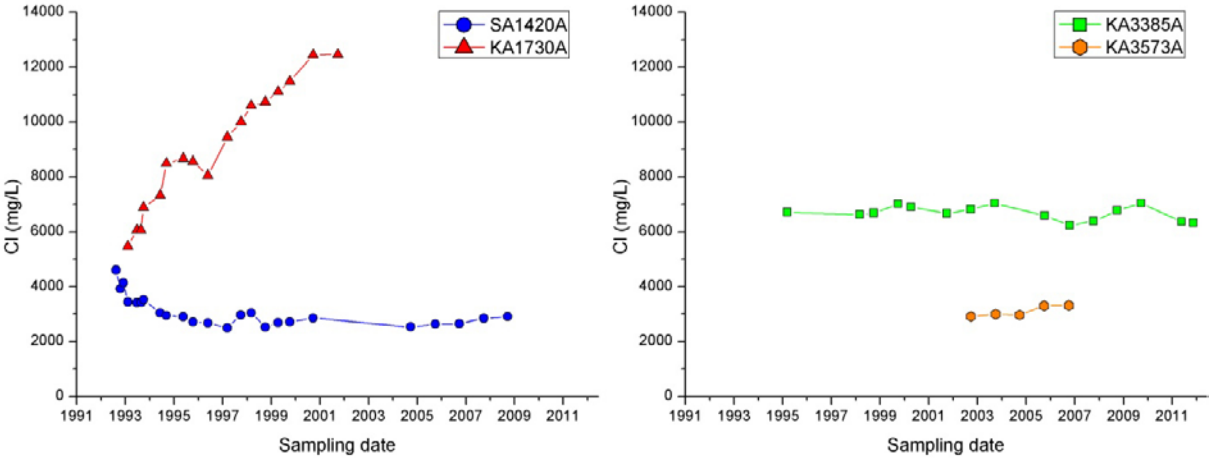

*Figure 7-1.* *Examples showing the evolution of the Cl concentration with time within different boreholes and sections. Left: changes in Cl concentration with time in the sample series collected in boreholes KA1420A and KA1730A. Right: in boreholes KA3385A and KA3573A, Cl concentrations in groundwater are generally stable over the monitored years.*

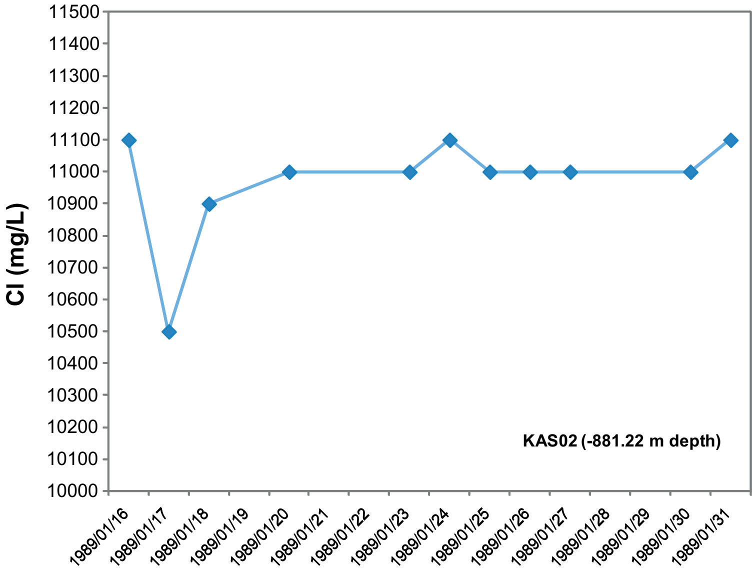

*Figure 7-2.* *Chloride time series in a section from borehole KAS02.*

### *Samples from the projects and experiments*

These samples refer to the group of samples stored in Data Set IV. The experimental or sampling procedures may have modified the groundwater chemistry and, therefore, it is uncertain if they can be used to characterise the system. However, depending on the purpose of the study they can be of use and are therefore kept in the excel file.

### *Samples from the weirs*

Although the main objective of the weir system is to monitor the water inflow along the different sections of the tunnel, electric conductivity and Cl concentration were also measured almost yearly in order to monitor the evolution of the water salinity with time. This information can be of use to get a general overview of the salinity along the 3,600 m long tunnel. It is noteworthy, however, that the values of these salinity parameters are representative of the water volume inside the weir. This water volume corresponds to the cumulative water flowing in a defined tunnel section (see Section 6.5 and Figures 6-2 and 6-3). The length of the different tunnel sections (length between two dams) varies greatly along the tunnel (Figure 6-2). Moreover, the water bearing fracture zones are inhomogeneously distributed along the tunnel with respect to length, width and water conductive properties etc. Accordingly, the salinity of the weir water may reflect the salinity of groundwater flushed out from the most conductive fractures of the studied tunnel section. In spite of the heterogeneity of the water conductive fractures, the general physicochemical parameters are relevant in the framework of a general characterisation considering the large range of salinity found in the fracture groundwater at Äspö HRL (e.g. Mathurin et al. 2012).

The sorting of the weirs according to their location along the four different parts of the tunnel (Figure 6-2) illustrates the spatial variation of the salinity (Figure 7-3 and Figure 7-4). Dissolved Cl was relatively low in the main ramp but varies substantially in the spirals and the bottom ramp. The maximum Cl concentration was measured in the second spiral, in weir MA2840G (Figure 7-3). In a more general context, the Cl concentrations in weir water are coherent with the spatial distribution of the Cl concentrations of fracture groundwater (Mathurin et al. 2012) where 1) values equivalent to the composition of the modern Baltic Sea were found in the main ramp, and 2) substantial concentration occurred in the northern part of the Äspö HRL. The values of electrical conductivity tend to be overall consistent with the Cl concentration.

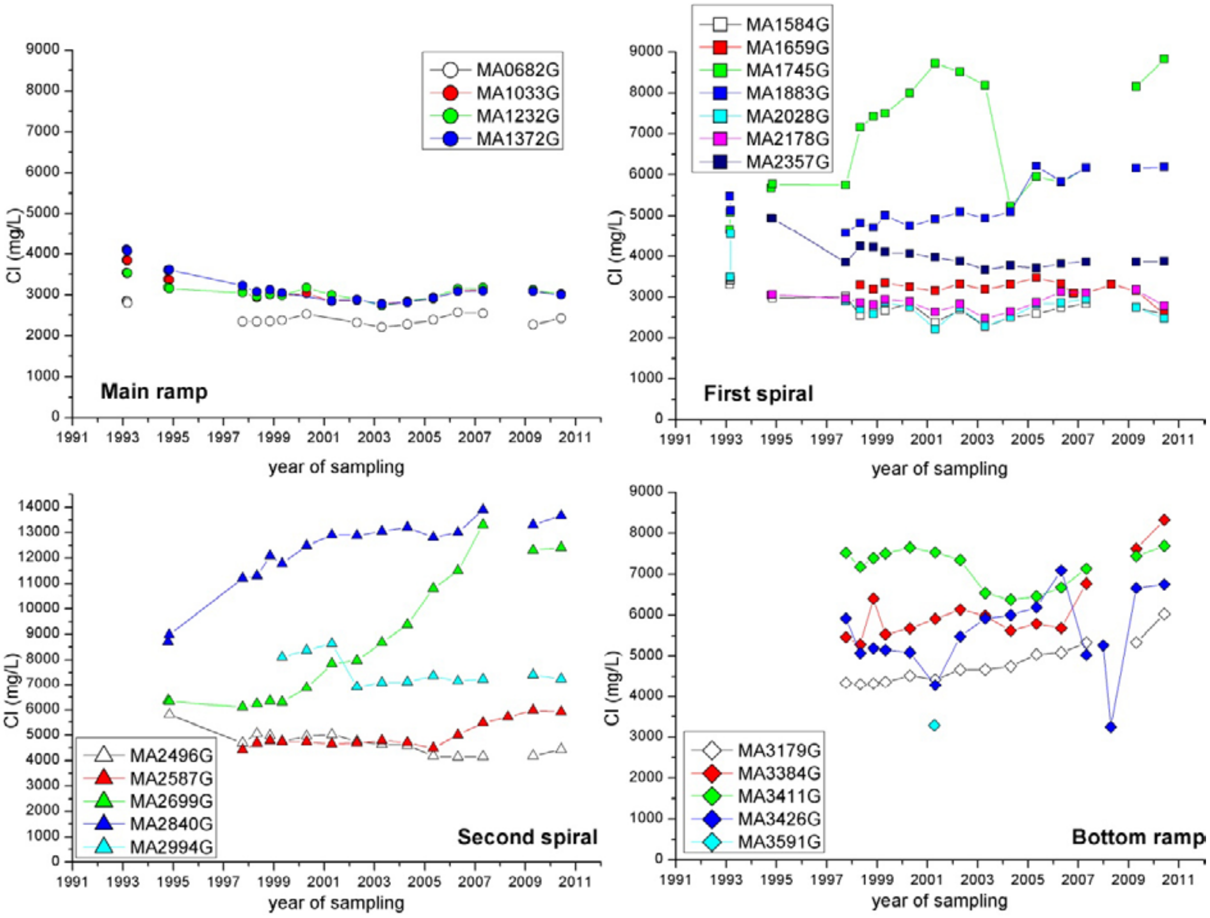

***Figure 7-3.*** *Evolution of Cl concentration collected in the weir system over the years. The weirs are organised by groups defined according to their location along the Äspö HRL: main ramp (top left), first spiral (top right), second spiral (bottom left) and bottom ramp (bottom right) defined in Figure 6-2 (Section 6.5).*

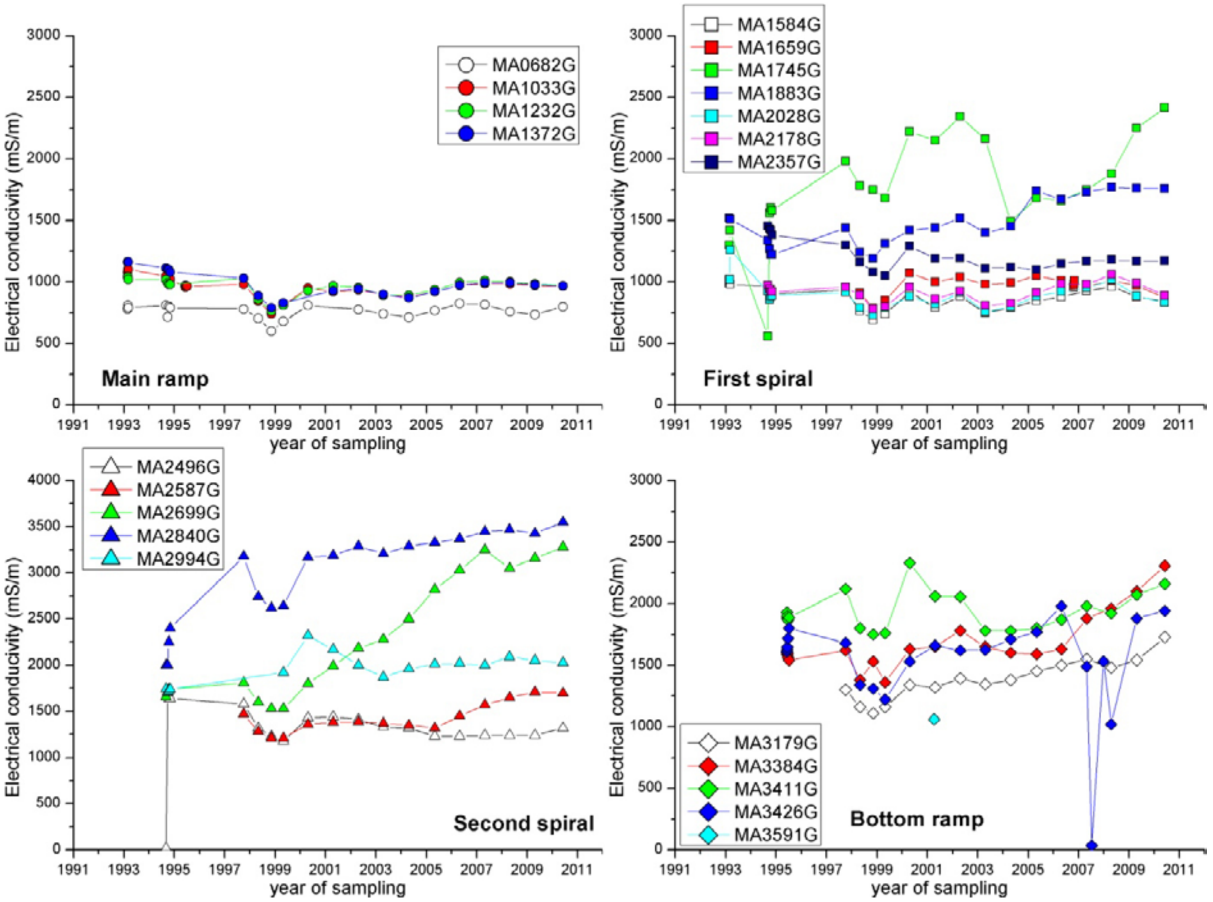

***Figure 7-4.*** *Evolution of the electrical conductivity of water collected in the weir system over the years. The weirs are organised by groups defined according to their location along the Äspö HRL: main ramp (top left), first spiral (top right), second spiral (bottom left) and bottom ramp (bottom right) defined in Figure 6-2.*

The temporal evolution of the Cl concentrations and the electrical conductivity of weir water highlight the variance of the values over time (Figure 7-3 and Figure 7-4). The overall evolution of the two parameters tends to illustrate the same general patterns. The change in Cl concentration found in the different parts of the tunnel with time is consistent with the hydraulic disturbances caused by the tunnel construction, for example 1) the rapid and prevailing intrusion of modern Baltic Sea in the main ramp, and 2) the up-coning of deep-lying saline groundwater described in fracture groundwater by Mathurin et al. (2012). However, an unexplained decrease of the electrical conductivity is observed in each of the weirs during the monitored period 1998–2000 (Figure 7-4). A possible artefact might have to be considered during the three year period when using the electrical conductivity parameter as this temporal trend cannot be identified in the Cl concentration.

### *Samples with microbial and gas data*

Most of the samples containing microbial and gas data correspond to specific experiments developed in the framework of specific projects. Most of the these samples do not have an equivalent sample chemically characterised but the microbe and gas content data could be very useful in comparative terms, or background information for other specific studies in the area or in similar sites.

When these data have been analysed in samples with a complete chemical characterisation, their use for modelling purposes is very important and makes that water sample an essential sample to describe the system.

### *Matrix pore-water samples*

There are 13 matrix pore-water analyses from six sections in one borehole from the Äspö HRL stored in the database that constitute useful information to increase knowledge concerning the origin of these rock matrix waters and to determine their possible influence on the chemistry of the fracture groundwaters.

The fracture groundwaters within a radius of several tens of metres surrounding the matrix borehole show evidence of large-scale groundwater movement through the bedrock during disturbed conditions (e.g. drawdown due to tunnel excavations) within the medium to high hydraulically active fractures. Over the range of transmissivity represented by these sampled fractures ($T=10^{-10}$ to $10^{-5}$ $m^2s^{-1}$), there is little obvious correlation between hydraulic properties and groundwater chemistry. In particular, this was clearly shown by most of the Prototype samples with one exception; KA3572G01 ($10^{-9}$ $m^2s^{-1}$) has been less influenced by the drawdown due to a longer response time which may reflect a different fracture orientation than the other sampled fractures. Drawdown effects are less evident from the 'J' Niche and also many of the TRUE Block Scale sites probably due to the sampling locations being further from the excavated tunnel system. Finally, groundwater compositions from boreholes KF0066A01 and KF0069A01 close to the experimental site, representing major water conducting sub-vertical fracture zones, represent the result of upconing of highly saline groundwaters typical of the deepest (~ 1,000 m) samples studied at Äspö.

In contrast, within the demarcated low transmissive site of the pore-water studies, access of groundwaters to the rock matrix is by flow through an interconnected network of fractures and microfractures characterised by ever decreasing hydraulic conductivities. Within the rock matrix itself, short-term solute transport (i.e. within the timescale of the matrix experiment) through the rock matrix is mainly by small-scale advection via a connecting network of microfractures and by diffusion. Analysis of the extracted rock matrix pore-waters (Sections 3 and 4, from borehole KF00051A011, see description in Section 3.2.5) show evidence of older dilute palaeogroundwaters preserved in the low hydraulically transmissive rock matrix. A component of matrix 'pore fluid' is also present. Section 2 from the same borehole appears to be anomalous suggesting some similarity with the Prototype samples which have been strongly influenced by a Baltic Sea drawdown. Access of this groundwater is probably via the close proximity (decimetres?) of a transmissive fracture of unknown dimensions.

Over repository timescales (i.e. hundreds to thousands of years) a greater contribution from diffusion of pore fluid/water from the rock matrix itself will be present since this will have had more time to undergo exchange by in- or out diffusion mechanisms depending on the nature of the chemical gradients existing between the microfracture groundwaters and the rock matrix pore fluids/waters. Generally at Äspö, permeable bedrock at all scales has facilitated the continuous removal and replacement of the interconnected pore space waters over relatively short periods of geological time, probably hundreds to a few thousands of years.

### *Samples from the regional area*

Finally, there is a set of data that will be very useful to put the Äspö system into a regional context in future modelling work. It is the data selected as representative from the Site Descriptive Modelling work in the Laxemar-Simpevarp area (133 samples of categories 1 to 4 in the SDM, Laaksoharju et al. 2009 and Tullborg et al. 2010b). These data can be found in SKBdoc 1393008.

## 7.2.1 Distribution of contents in the final data set

As indicated in previous chapters, the data that are suitable for modelling purposes are those belonging to categories 1 to 3 and, although with some caution, also categories 3b and 4 (all included in Data Set I); however, for a general idea of the system, Category 5 samples (Data Set II) are also useful. Bearing this in mind, Figures 7-5 to 7-10 show the general distribution of contents in these groundwaters (included in Data sets I and II) with respect to depth and chloride; only the major ions and $\delta^{18}O$ have been plotted.

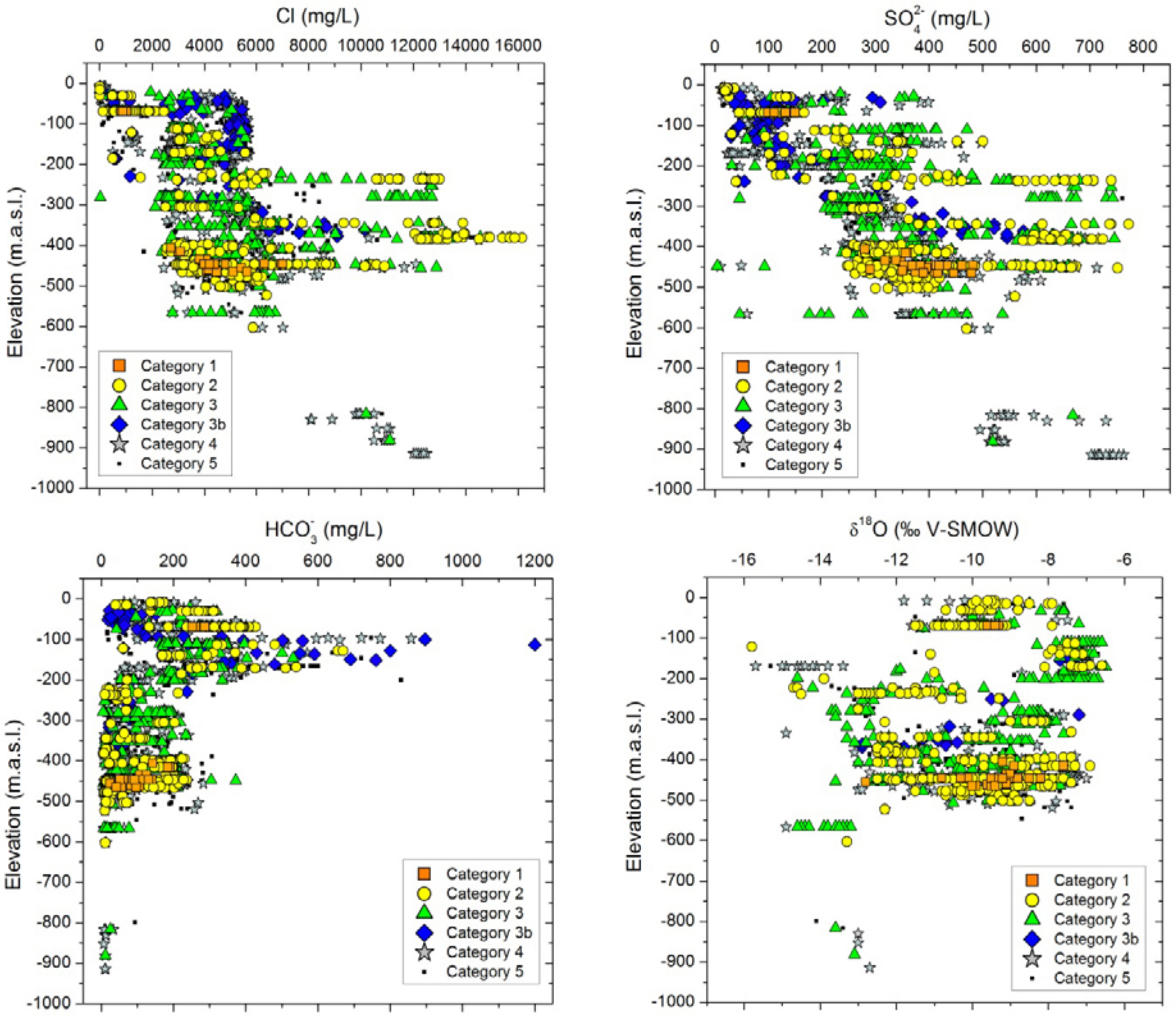

***Figure 7-5.*** *General distribution of chloride (a), sulphate (b), bicarbonate (c) and $d^{18}$O (d) with depth, in the samples included in Data Sets I and II.*

Due to the high number of samples available (2,259), many of them plot superimposed on each other. In the following figures, the better categories are shown in the first planes in such a way that there are very few Cat. 4 and Cat. 5 samples to be seen in the plots. Obviously, most of them occur just underneath the rest of the better quality samples, but this fact is quite important as it indicates that even these samples are in the same range as the others. As indicated previously, most of the low category samples have been allocated low grades because of insufficient information, not because the data were unreliable, but simply there is not enough information to be certain one way or another.

Distribution of major anions and cations with depth is similar to that found previously in the other studied sites in Sweden (Laaksoharju et al. 2008, 2009, Nilsson et al. 2011): a general increase in chloride, sulphate, sodium and calcium and a general decrease in bicarbonate, magnesium and potassium. The main difference is the broader range of variation in the contents at almost all depths.

Even if this is clearly the result of disturbances in the system over the 25 years of sampling, this wide range of values can also be seen during shorter periods of time, indicating that the variability of the chemistry in the system is quite high. This has been plotted in Figures 7-7 and 7-8. Different colours and symbols have been used for four different periods of time: a) samples representative of the initial conditions (previous to the tunnel construction or just while it was being excavated, from 1987 to 1995), b) samples taken over the construction period between 1990 and 1995; c) samples taken during the operational phase from 1996 until 2007, and d) samples taken in the last years, from 2008 to 2011 (to specifically show the present situation).

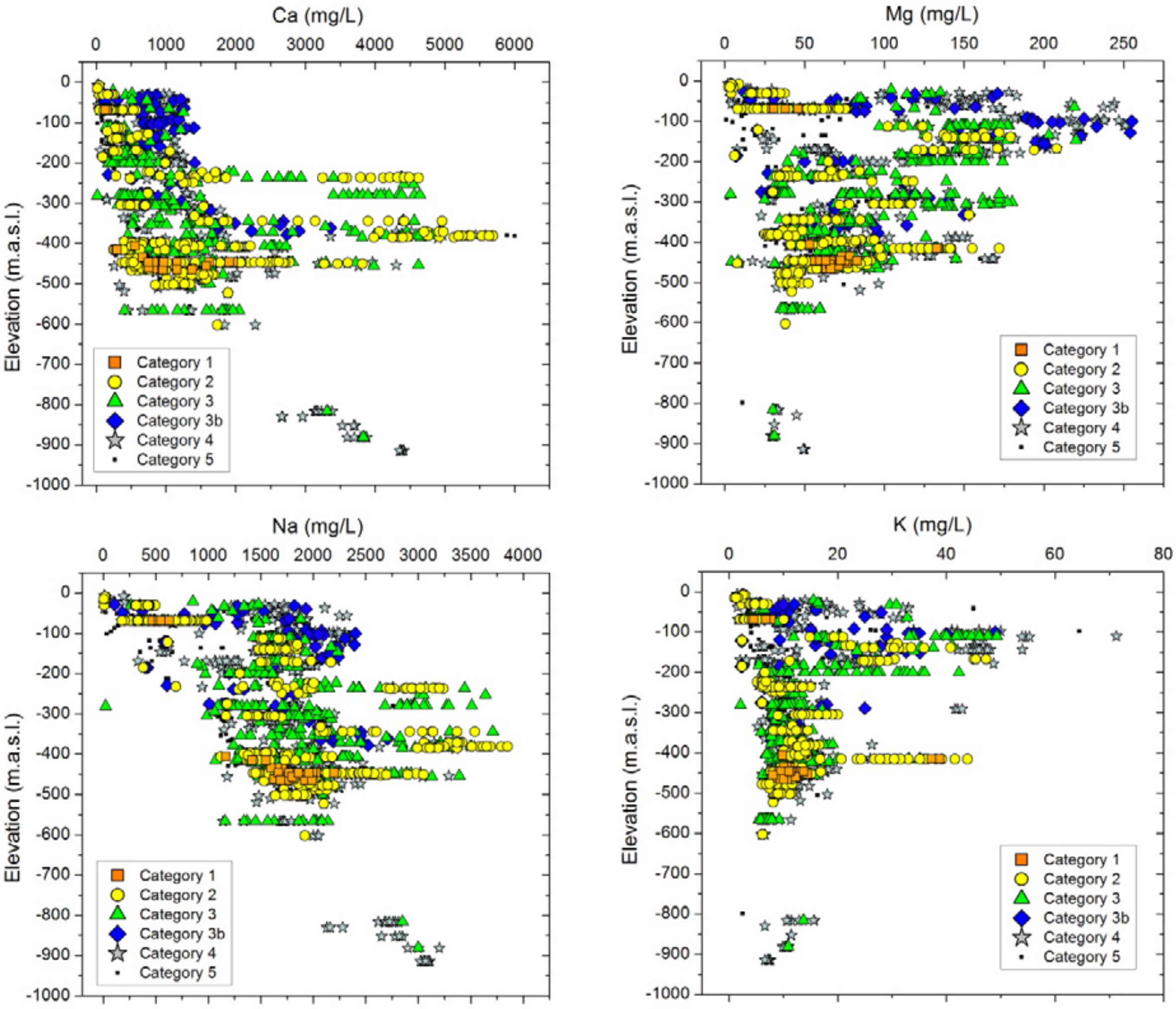

***Figure 7-6.*** *General distribution of calcium (a), magnesium (b), sodium (c) and potassium (d) with depth, in the samples included in Data Sets I and II.*

Quite a broad range of contents for some elements is already seen in the samples considered representative of the initial conditions (cyan circles in the plots). In general, they show a wide variation in all the contents at almost all depths down to –400 m although not as broad as the samples taken later in time. Some exceptions will be commented below. Deeper down, the number of samples taken before tunnel construction is very few and they do not cover any of the ranges of contents covered by the samples taken after the tunnel construction. An exception to this is the fact that almost all the deepest samples (800 m to 1,000 m depth) correspond to this initial condition group (except for some taken during the construction phase; see dark grey triangles in the plots).

The group of samples taken during the construction phase expands their range of contents, but not very much, with respect to the initial conditions. Then, the final other two groups, which represent the operation phase period, are very similar and show in general the same situation during a period of 16 years, the highest ranges of variations for almost all the elements.

There is an additional factor affecting the distribution of the contents with depth and it is the location (in time and space) of the different projects and experiments. In general, there are more groundwater samples taken at specific depths due to the specific objectives of the different projects. A clear example is the number of samples taken at the repository depth (between –400 and –500 m).

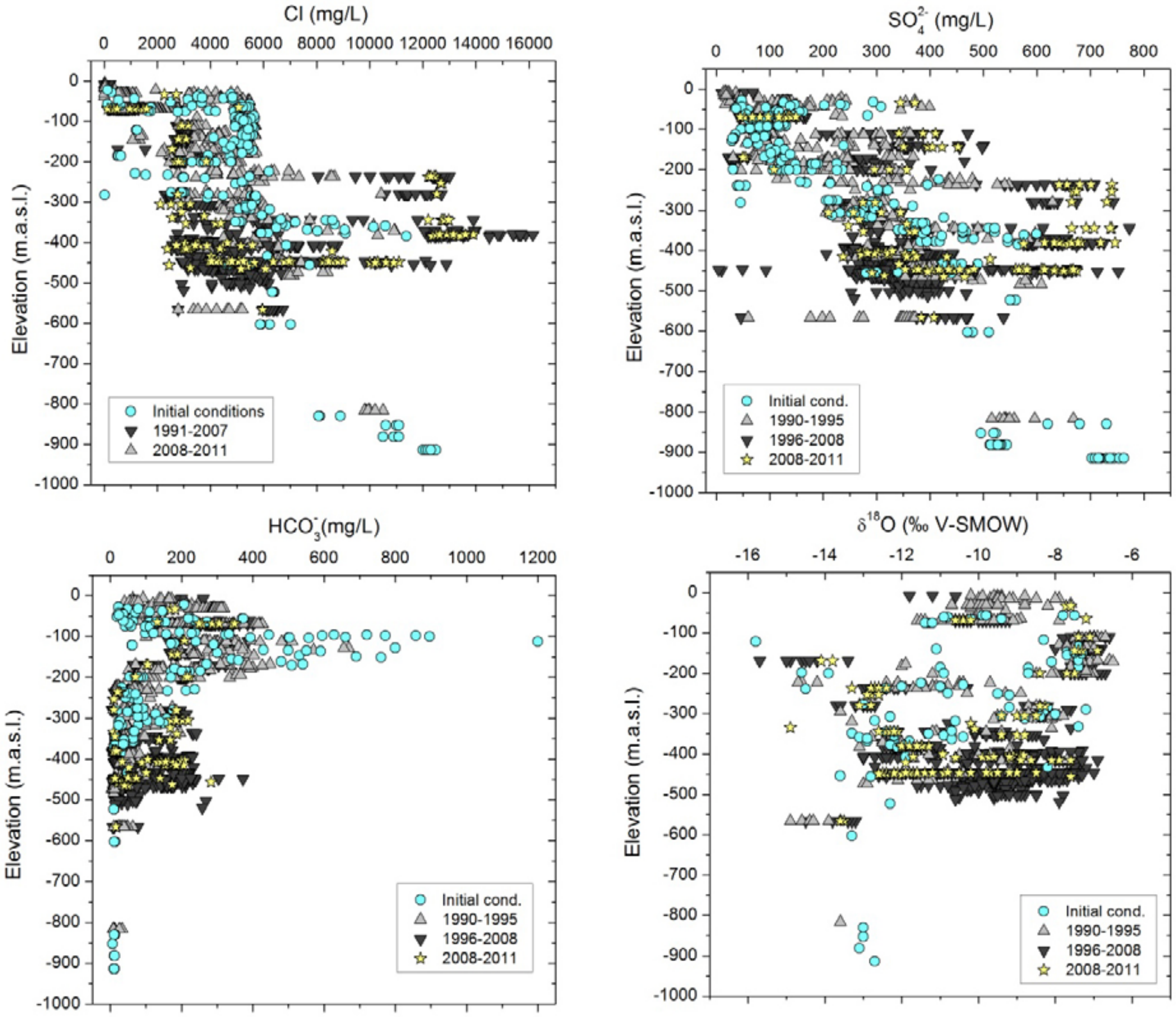

***Figure 7-7.*** *Ranges and distribution of the main anion contents and the d*$^{18}$*O values at different periods of time: Initial conditions, from 1990 to 1995, from 1996 to 2007 and from 2008 to 2011.*

Even not being the objective of this report, these plots and the following plots showing the distribution of the elements with respect to chloride, provide a very interesting view of the behaviour of the system and the effects of the disturbances on the groundwater types in time and space. Some immediate observations include:

- Increase in chloride after the tunnel construction clearly marked at 400 m depth (but affecting also groundwaters between 250 and 450 m depth) and slight decrease in the latest samples (yellow stars) although still with contents higher than before and during the tunnel construction.
- Special characters and evolution of groundwaters located mainly between –100 and –200 m but in some cases down to –400 m depth. The initial conditions show: 1) more or less constant chloride content at around 5,500 mg/L, 2) low sulphate content, 3) extremely high content of bicarbonate, 4) the highest magnesium concentrations, and 5) calcium and sodium contents higher than in the rest of the samples from the same depths. This special character disappears after the beginning of the tunnel construction and the evolution of these waters with time shows, in general, a decrease in all the components except in Sulphate, which increases.
- $\delta^{18}O$ shows a broad range of values at almost all depths and almost at any time.

The distribution of the major ions with respect to chloride is shown in figures 7-9 and 7-10. The same temporal code just seen in the plots with depth is used here. The general evolution is coherent with the fact that, in general, chloride increases with depth, therefore, sulphate, calcium and sodium increase with chloride, while bicarbonate, magnesium and potassium decrease.

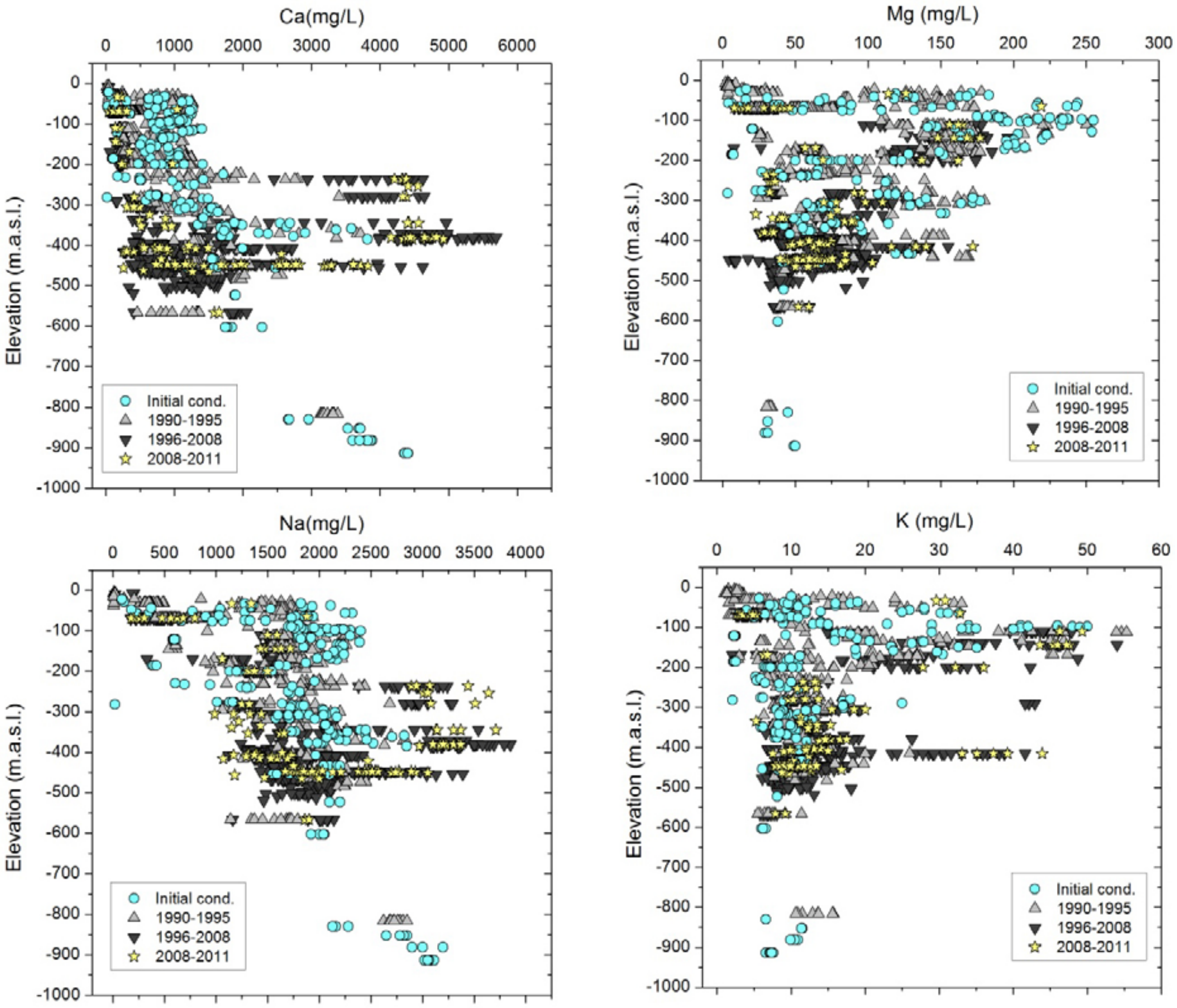

***Figure 7-8.*** *Ranges and distribution of the main cation contents at different periods of time: Initial conditions, from 1990 to 1995, from 1996 to 2007 and from 2008 to 2011.*

However, although these are the general trends, there are some indications of special groundwater characters and evolution that will give additional clues to what has been observed above. In order to have a better idea about the water types, the end members that have been used in all the previous site characterisation studies are also shown in the next plots (Laaksoharju et al. 2008, 2009).

- Calcium and sodium contents follow the general trend of increasing values with chloride content and no special differences can be seen with time. Something similar happens with the values of $\delta^{18}O$. The distribution of values is more or less similar with time except for the fact that only the initial conditions could be described as being to closer to the Littorina end member, while samples taken after the tunnel construction are closer to the Baltic isotopic signature.
- Magnesium and potassium are more interesting as they show a clear difference in behaviour before and during the tunnel construction, and the rest of the waters taken after tunnel construction. Waters from the initial conditions and some of the waters taken during the tunnel construction show a clear peak in Mg and K contents towards the Littorina end member, and just around a chloride content of 5,500 mg/L. With time, groundwaters move towards another peak with lower Mg, K and Cl contents typical of the Baltic Sea end member.
- Bicarbonate shows a similar behaviour as its contents in the initial conditions are much higher than in the rest of the groundwater samples, and these values are also associated with chloride contents around 5,500. Sulphate behaves in parallel with the lowest values measured in the system, associated with those waters with high bicarbonate. Both facts are coherent with a series of geochemical process that could have taken place in the sea sediments during the Littorina period (Gimeno et al. 2009).

In summary, there is a clear indication of the Littorina presence in the system just before the tunnel construction and the progressive dilution (mainly due to intrusion of present Baltic Sea water) of that signature over time. This is mainly seen in the samples located between 100 and 200 m depth but also in some of the boreholes at around 400 m depth.

In contrast, other boreholes show higher salinity than during initial conditions, which is interpreted as the result of up-coning. This is most evident in the northern and north-western part of the tunnel spiral. The fact that some structures (and thereby some borehole sections) show up-coning of saline water whereas some other structure show intrusion of Baltic Sea water at the same depth (but mainly in the south-eastern part of the tunnel spiral), explains the large spread in Cl, Na and Ca and many other species seen in Figure 7-9.

All this will be the subject of future modelling work on the hydrogeochemistry of the Äspö system.

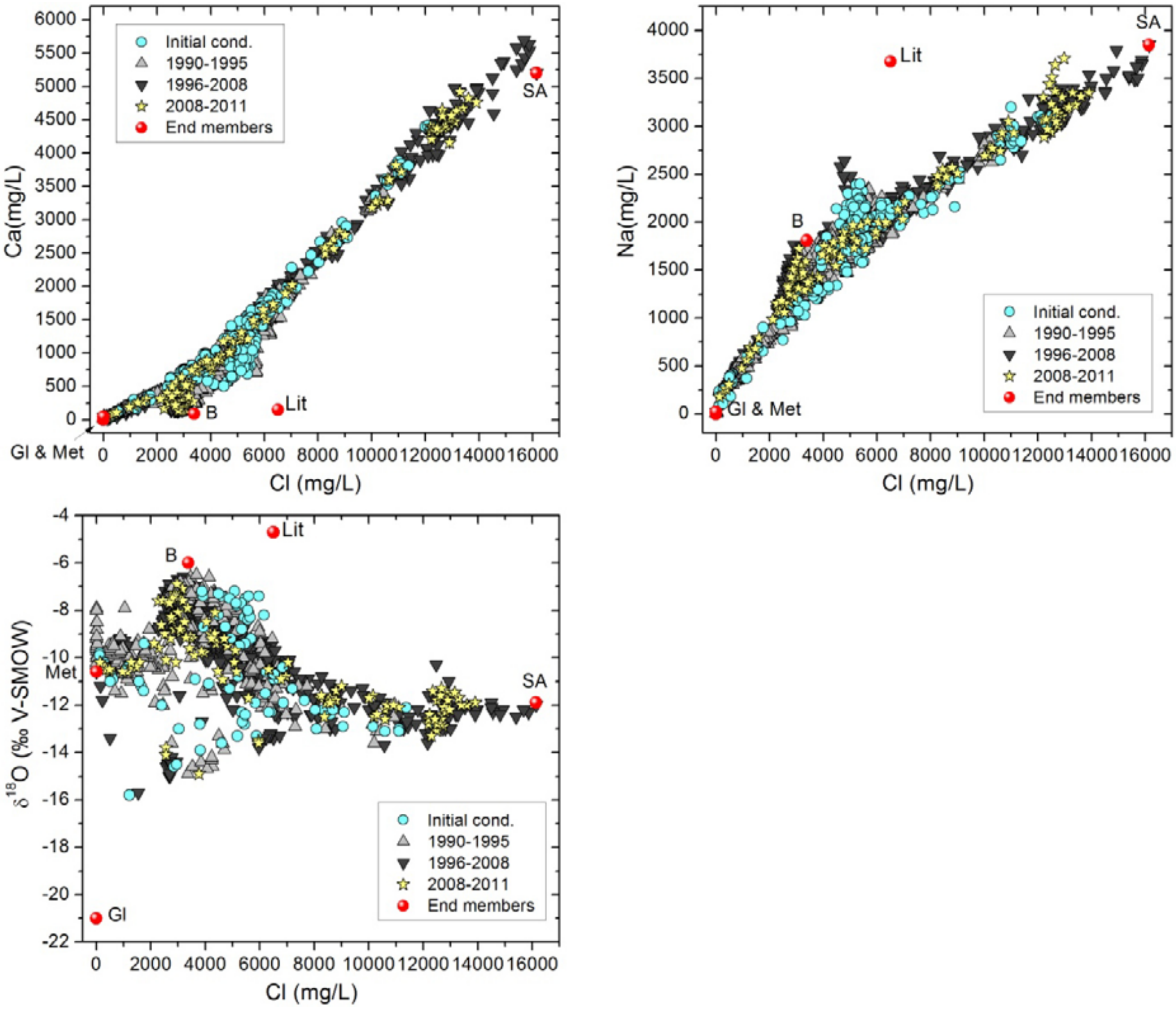

***Figure 7-9.*** *General distribution of calcium (a), sodium (b), and* $\delta^{18}O$ *values (c) with chloride, in samples included in Data Sets I and II. The corresponding position of the end-member waters used in the previous site description works are also shown: Met (meteoric), B (Baltic), Lit (Littorina), Gl (Glacial) and SA (Saline water from Äspö; see Mathurin et al. 2012).*

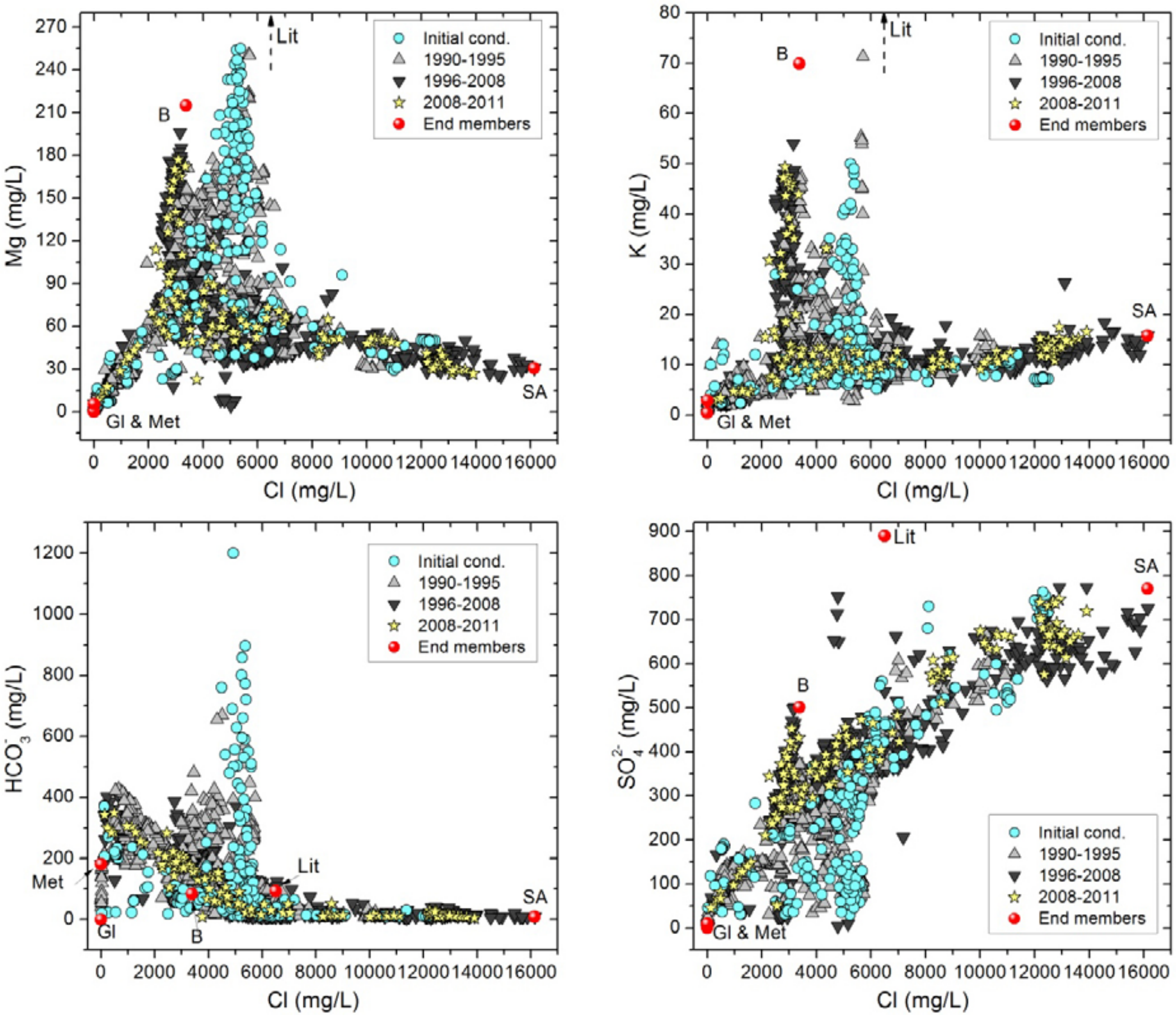

***Figure 7-10.*** *General distribution of magnesium a), potassium b), bicarbonate c) and sulphate d) with chloride, in the samples included in Data Sets I and II. The corresponding position of the end-member waters used in the previous site description works are also shown: Met (meteoric), B (Baltic), Lit (Littorina), Gl (Glacial) and SA (Saline water from Äspö; see Mathurin et al. 2012).*

# 8 Experiences and possible improvements

Being a data report the conclusions about the data correspond to the final set of selected samples and their quality, which has already been presented in Chapter 7. This last chapter summarises, as a sort of conclusions, the main lessons learnt while performing the work presented in this report with special emphasis on the strategies recommended for the future.

## 8.1 General

The hydrochemical dataset from Äspö constitutes unique material for well founded groundwater modelling due to the length of the sampling period, the number of samples, the often extensive analyses and the generally good data quality. Furthermore, the amount of supportive data from other geoscientific disciplines and from the operation of the facility make the integration with geology and hydrogeology easier in order to obtain consistency in the different descriptions. The data evaluation in the present report have resulted in a well structured dataset (1,585 samples in Dataset I) containing quality categorised data of high quality for general interpretation and modelling purposes, a minor dataset with rejected data (674 samples in Dataset II) and a few additional datasets containing data that may be used with caution for other special purposes.

Although the quality categorisation of each sample is not a straightforward and obvious procedure, it is believed that the categorisation as presented in Figure 5-5 provides a good general idea of the quality of the dataset and of each included sample, which will be useful for future modeling exercises. The quality categories allocated to the samples in Dataset I reflects the completeness of the analyses and, to some extent, the performance of the sampling method, rather than the quality of the analyses. However, a sample with incomplete analyses cannot be evaluated in all the aspects so the analytical quality may be more uncertain for this sample and it will also be less useful for modelling purposes.

Some issues and aspects which were not, or only sparsely, treated in the latest interpretation and modelling exercises at Äspö (Geomod 2002) (Laaksoharju and Gurban 2003) and whose understanding has improved later on, should be considered in future modelling exercises.This has been taken into account when presenting the report and structuring the data tables. For example;

- Correlation between groundwater composition and geological entities/structures and their hydraulic properties were discussed in the Forsmark and Laxemar SDMs (SKB 2008, 2009). Further knowledge was gained from the very heterogeneous groundwater composition and hydraulic properties revealed in the SFR-extension project (SKB 2011). The smaller scale and the small distances between data points/sampling locations facilitated the understanding of the SFR groundwater system. The integrated modelling of the Äspö data may supply important complementary information. The scale is the same as for the SFR but the conditions are slightly different, for example the hydraulic contact is mainly vertical in contrast to the SFR where the contact is horizontal. The differences and similarities between the groundwater systems at Äspö HRL, SFR, Forsmark, and Laxemar may contribute to a better general understanding of groundwater formation and groundwater flow paths in crystalline systems.
- Changes in the groundwater composition are caused by the presence of a tunnel (up-coning, meteoric or Baltic water intrusion, increased mixing of different water types) due to its impact on the hydraulic conditions. Where and how these changes appear and the correlation to geological entities/structures and their hydraulic properties, give information comparable to hydraulic tracer tests.
- Differentiation between marine groundwaters of Littorina and Baltic origin.
- Decreasing inflow with time to tunnel systems and chemical composition of the inflowing water.

## 8.2 Investigation programmes and sampling strategies

The data evaluation work has revealed some shortcomings that reflect the different investigation programmes and the sampling strategies during the investigation period (1988–2011):

- Lack of – or few data
  When evaluating groundwater data obtained as far back as 20 to 30 years ago, a frequently recurrent problem is that strategic samples have incomplete sets of data or lack the most important analytical value that could have answered a critical question. This may be due to logistic or cost reasons and stresses the importance of foreseeing as many implications as possible when planning future hydrochemical sampling programmes. Furthermore, in the Äspö HRL case there are special samples that have been collected for rare and sophisticated analyses or determinations but the basic groundwater composition has not been analysed for the same samples. This is generally due to the specific nature and purpose of the sample/experiment. However, had the basic groundwater analyses been included, the samples would have been useful also for many other modelling purposes.
- Lack of – or few early/initial samples with complete data
  Documentation of the initial hydrochemical conditions is especially important during tunnel construction (Äspö HRL, the earlier SFR, and also the future repository for nuclear waste in Forsmark). They set the original system state unaffected by the changes in the hydraulic conditions due to the tunnel excavation. In the Äspö HRL case the surface borehole data from the pre-investigation phase gave valuable information and the regularly drilled probing boreholes (sampled in between the blasting rounds) may also be considered as relatively unaffected by the tunnel at the first sampling occasion. However, probably due to time constraints the analytical protocol for these initial samples did not include any isotopes. In retrospect, data on $\delta^{18}O$ (‰ V-SMOW) would have been very useful.
- Too few continuous sample series are available, covering the entire time period between the drilling of the borehole and present date. Long sample series without too many breaks are important in order to follow the changes in water composition due to tunnel construction and to understand the system, i.e. what kind of changes appear, where and at what velocity. This information can be regarded as similar to what is obtained by hydraulic tracer test and is useful also for the hydrogeologists.
- Ideally, the data should be used for modelling purposes relatively close in time (one or two years at most) after they have been obtained and stored in the database. In that way errors and inconsistencies are easily found, the performance and possible incidents are still remembered and it may also give the possibility to modify the investigation programme if motivated by the results. This has not always been the case at Äspö and it is especially important when data are obtained in monitoring programmes that are extended in time.

It will never be possible or even desirable to analyse all the components listed in the "SKB tool box" (see Table 3-1) in all samples, as the groundwater samples are originally collected for very different purposes. The most incomplete samples in the Äspö HRL dataset have been taken for simple and quick checks of some parameters such as pH or salinity. Typical examples are checks of impacts from grouting and sampling of inflowing water to the weirs and consequently they are generally analysed for very few parameters (pH and possibly $HCO_3$, chloride or EC). In retrospect, more complete analyses of these samples would have facilitated interpretation of the impact of grouting on the groundwater composition and of the composition of the inflowing water to different tunnel segments, respectively. There may be many other reasons to include more parameters also for additional samples that are known to be not representative of the undisturbed groundwater conditions in the bedrock, in order to increase knowledge about the disturbed situation.

Furthermore, many of the early Äspö HRL samples lack all or some of the isotopes. There should be a recommended minimum set of analyses to describe the initial distribution and changes with time in terms of groundwater salinity and/or groundwater types and these should include major components and the isotopes $\delta^{18}O$ ‰ V-SMOW, $\delta^{2}H$ ‰ V-SMOW and $^{3}H$ (TU). In the case of long time series, for samples collected during continuous discharge from the borehole section being sampled, the isotope determinations may be omitted for many of the samples, if the basic groundwater composition is stable.

## 8.3 Data storage and documentation

The present data evaluation as well as the previous evaluation of the SFR-extension dataset (Nilsson 2011) concerns data gathered during a very long time period (about 25 years). Possible future evaluations of the Forsmark data, including present data as well as data from the ongoing long term monitoring and the future detailed investigations during the construction phase of the planned repository, will probably imply similar or longer time periods. A general impression from the combined Äspö and SFR examples is that despite the fact that databases, database structures, database administrators and investigation and modelling, personal may have changed during the years the data are generally stored and documented correctly in a logical and understandable way. The major inconsistencies and errors observed are described briefly in Section 7.1.2. Some possible improvements or other important factors to consider are:

- The early data were stored at a time when it was important to minimise the volume of stored data since the capacity of the database was limited; this implied that only good quality data were evaluated and stored. Analyses and measurements that were judged to be erroneous at that time, as well as unrepresentative samples, were omitted. At present (since the tunnel construction and the introduction of the Sicada database) every sample and result is now stored in the Sicada database, even those analyses of poor quality. The Äspö Dataset contains data according to both strategies which has both advantages and disadvantages. In the early approach, even though there is less doubt about the data there is a risk for misjudgement and correct values or samples may be rejected just because they are unexpected. In the latter case, due to the number of samples and data, the data volume becomes very large and heterogeneous from the quality aspect. Possibly, some kind of quality classification could be introduced already at this stage in the database to facilitate sorting out useful data.
- A time consuming task in the data evaluation work has been to sort out samples representing normal sampling conditions (including samples impacted by the hydraulic situation due to the tunnel) from samples influenced by special experimental conditions. It is most probable that too many samples have been included in Dataset IV just due to uncertainty. The different experiments in Äspö HRL are partly the reason for the somewhat deteriorating hydrochemistry structure in the Sicada database today. It is suggested that it should be possible (easier than today) to separate data from general sampling programmes, including the basic components according to Table 3-1, from data generated in projects with special experimental conditions and/or parameters.
- There is a need for a well organised database structure and a stricter control and checking protocol before adding new tables, columns or parameters. Furthermore, more discussions between the database administrators and the end users of the Sicada database would be beneficial for further development of Sicada, or even a new database to replace Sicada in future detailed investigations in Forsmark.
- The number of reports with detailed documentation of the work done at Äspö during the pre-investigations as well as later on in the Äspö HRL is very impressive and much information is available although it may be time consuming to find it. For example, in some cases there may be a need to integrate and compare several reports. Information that has been difficult to extract from reports and from Sicada includes 1) the dates when changes of analytical methods, detection limits and measurement uncertainties have been implemented, as well as what were the old and new values for detection limits and measurement uncertainties, and 2) details concerning the sampling methods, for example exchanged water volumes prior to sampling or sampling direction from the borehole section (e.g. which tube was used as an outlet for the sampled water) when sampling in tunnel boreholes. The last point has implications, for example when assessing sulphide concentrations.

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### Unpublished documents

| SKBdoc id, version | Title | Issuer, year |
|---|---|---|
| 1393008 ver 1.0 | Äspö Data Report | SKB, 2013 |

# Appendix 1

## Detection/reporting limits and measurement uncertainties

**Table A1-1. Reporting limits and measurement uncertainties – updated 2008.**

| Component | Method[1] | Reporting limits (RL), detection limits (DL) or range[2] | Units | Measurement uncertainty[3] |
|---|---|---|---|---|
| pH | Potentiometric | 3–10 | pH unit | ±0.1 |
| EC | Electrical Conductivity measurement | 1–150<br>150–10,000 | mS/m | 5%<br>3% |
| $HCO_3$ | Alkalinity titration | 1 | mg/L | 4% |
| $Cl^-$<br>$Cl^-$ | Mohr-titration<br>IC | ≥ 70<br>0.5 – 70 | mg/L | 5%<br>8% |
| $SO_4$ | IC | 0.5 | mg/L | 12% |
| $Br^-$ | IC | DL 0.2, RL 0.5 | mg/L | 15% |
| Br | ICP SFMS | 0.001, 0.004, 0.010[4] | mg/L | 25%[5] |
| $F^-$<br>$F^-$ | IC<br>Potentiometric | DL 0.2, RL 0.5<br>DL 0.1, RL 0.2 | mg/L | 13%<br>12% |
| $I^-$ | ICP SFMS | 0.001, 0.004, 0.010[4] | mg/L | 25%[5] |
| Na | ICP AES | 0.1 | mg/L | 13% |
| K | ICP AES | 0.4 | mg/L | 12% |
| Ca | ICP AES | 0.1 | mg/L | 12% |
| Mg | ICP AES | 0.09 | mg/L | 12% |
| S(tot) | ICP AES | 0.16 | mg/L | 12% |
| Si(tot) | ICP AES | 0.03 | mg/L | 14% |
| Sr | ICP AES | 0.002 | mg/L | 12% |
| Li | ICP AES | 0.004 | mg/L | 12.2% |
| Fe | ICP AES | 0.02 | mg/L | 13.3%[6] |
| Fe | ICP SFMS | 0.0004, 0.002, 0.004[4] | mg/L | 20%[6] |
| Mn | ICP AES | 0.003 | mg/L | 12.1%[5] |
| Mn | ICP SFMS | 0.00003, 0.00004, 0.0001[4] | mg/L | 53%[6] |
| Fe(II), Fe(tot) | Spectrophotometry | DL 0.006, RL 0.02 | mg/L | 0.005 (0.02–0.05 mg/L)<br>9% (0.05–1 mg/L)<br>7% (1–3 mg/L) |
| $HS^-$ | Spectrophotometry, SKB | SKB DL 0.006, RL 0.02 | mg/L | 25% |
| $HS^-$ | Spectrophotometry, external laboratory | 0.01 | mg/L | 0.02 (0.01–0.2 mg/L)<br>12% (> 0.2 mg/L) |
| $NO_2$ as N | Spectrophotometry | 0.1 | μg/L | 2% |
| $NO_3$ as N | Spectrophotometry | 0.2 | μg/L | 5% |
| $NO_2$+$NO_3$ as N | Spectrophotometry | 0.2 | μg/L | 0.2 (0.2–20 μg/L)<br>2% (> 20 μg/L) |
| $NH_4$ as N | Spectrophotometry, SKB | 11 | μg/L | 30% (11–20 μg/L)<br>25% (20–50 μg/L)<br>12% (50–1,200 μg/L) |
| $NH_4$ as N | Spectrophotometry external laboratory | 0.8 | μg/L | 0.8 (0.8–20 μg/L)<br>5% (> 20 μg/L) |
| $PO_4$ as P | Spectrophotometry | 0.7 | μg/L | 0.7 (0.7–20 μg/L)<br>3% (> 20 μg/L) |
| $SiO_4$ | Spectrophotometry | 1 | μg/L | 2.5% (> 100 μg/L) |
| $O_2$ | Iodometric titration | 0.2 – 20 | mg/L | 5% |
| Chlorophyll a, c pheopigment[7] | /1/ | 0.5 | μg/L | 5% |

| Component | Method[1] | Reporting limits (RL), detection limits (DL) or range[2] | Units | Measurement uncertainty [3] |
|---|---|---|---|---|
| PON[7] | /1/ | 0.5 | µg/L | 5% |
| POP[7] | /1/ | 0.1 | µg/L | 5% |
| POC[7] | /1/ | 1 | µg/L | 4% |
| Tot-N[7] | /1/ | 10 | µg/L | 4% |
| Tot-P[7] | /1/ | 0.5 | µg/L | 6% |
| Al, | ICP SFMS | 0.2, 0.3, 0.7[4] | µg/L | 17.6%[6] |
| Zn | ICP SFMS | 0.2, 0.8, 2[4] | µg/L | 15.5, 17.7, 25.5%[6] |
| Ba, Cr, Mo, | ICP SFMS | 0.01, 0.04, 0.1[4] | µg/L | Ba 15%[4], Cr 22%[5] Mo 39%[6] |
| Pb | ICP SFMS | 0.01, 0.1, 0.3[4] | µg/L | 15%[6] |
| Cd | ICP SFMS | 0.002, 0.02, 0.5[4] | µg/L | 15.5%[6] |
| Hg | ICP AFS | 0.002 | µg/L | 10.7%[6] |
| Co | ICP SFMS | 0.005, 0.02, 0.05[4] | µg/L | 25.9%[6] |
| V | ICP SFMS | 0.005, 0.03, 0.05[4] | µg/L | 18.1%[6] |
| Cu | ICP SFMS | 0.1, 0.2, 0.5[4] | µg/L | 14.4%[6] |
| Ni | ICP SFMS | 0.05, 0.2, 0.5[4] | µg/L | 15.8%[6] |
| P | ICP SFMS | 1, 5, 40[4] | µg/L | 16.3%[6] |
| As | ICP SFMS | 0.01 (520 mS/m) | µg/L | 59.2%[6] |
| La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu | ICP SFMS | 0.005, 0.02, 0.05[4] | µg/L | 20%, 20%, 25%[6] |
| Sc, In, Th | ICP SFMS | 0.05, 0.2, 0.5[4] | µg/L | 25%[6] |
| Rb, Zr, Sb, Cs | ICP SFMS | 0.025, 0.1, 0.25[4] | µg/L | 15%, 20%, 20%[5]<br>25%[6] |
| Tl | ICP SFMS | 0.025, 0.1, 0.25[4] | µg/L | 14.3%[5 and 6] |
| Y, Hf | ICP SFMS | 0.005, 0.02, 0.05[4] | µg/L | 15%, 20%, 20%[5]<br>25%[6] |
| U | ICP SFMS | 0.001, 0.005, 0.01[4] | µg/L | 13.5%, 14.3%, 15.9%[5]<br>19.1%, 17.9%, 20.9%[6] |
| DOC | UV oxidation, IR detection Carbon analysator | 0.5 | mg/L | 8% |
| TOC | UV oxidation, IR detection Carbon analysator | 0.5 | mg/L | 10% |
| $\delta^{2}$H | MS | 2 | ‰ SMOW[8] | 0.9 (one standard deviation) |
| $\delta^{18}$O | MS | 0.1 | ‰ SMOW[8] | 0.1 (one standard dev.) |
| $^{3}$H | LSC | 0.8 | TU[9] | 0.8 |
| $\delta^{37}$Cl | A (MS) | 0.2 | ‰ SMOC[10] | 0.2[17] |
| $\delta^{13}$C | A (MS) | – | ‰ PDB[11] | 0.3[17] |
| $^{14}$C pmc | A (MS) | – | PMC[12] | 0.4[17] |
| $\delta^{34}$S | MS | 0.2 | ‰ CDT[13] | 0.4 (one standard dev.) |
| $^{87}$Sr/$^{86}$Sr | TIMS | – | No unit (ratio)[14] | 0.00002 |
| $^{10}$B/$^{11}$B | ICP SFMS | – | No unit (ratio)[14] | – |
| $^{234}$U, $^{235}$U, $^{238}$U, $^{232}$Th, $^{230}$Th | Alfa spectr. | 0.0001 | Bq/L[15] | ≤ 5% (Counting statistics uncertainty) |
| $^{222}$Rn, $^{226}$Ra | LSS | 0.015 | Bq/L | ≤ 5% (Counting statistics uncertainty) |

1. Many elements may be determined by more than one ICP technique depending on concentration range. The most relevant technique and measurement uncertainty for the concentrations normally encountered in groundwater are presented. In cases where two techniques were frequently used, both are displayed.

2. Reporting limits (RL) are generally 10×standard deviation if nothing else is stated. Measured values below RL or DL are stored as negative values in SICADA (i.e. –RL value and –DL value).

3. Measurement uncertainty reported by the laboratory is generally as ± percent of measured value in question at 95% confidence interval.

4. Reporting limits at electrical conductivity 520 mS/m, 1,440 mS/m and 3,810 mS/m respectively.

5. Measurement uncertainty at concentrations 100×RL.

6. Measurement uncertainty at concentrations 10×RL.

7. Determined only in surface waters. PON, POP and POC refers to Particulate Organic Nitrogen, Phosphorous and Carbon, respectively.

8. Per mille deviation16 from SMOW (Standard Mean Oceanic Water).

9. TU=Tritium Units, where one TU corresponds to a tritium/hydrogen ratio of 10–18 (1 Bq/L Tritium=8.45 TU).

10. Per mille deviation16 from SMOC (Standard Mean Oceanic Chloride).

11. Per mille deviation16 from PDB (the standard PeeDee Belemnite).

12. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age:
pmC=100 × e((1,950-y-1.03t)/8,274) where y=the year of the C-14 measurement and t=C-14 age.

13. Per mille deviation16 from CDT (the standard Canyon Diablo Troilite).

14. Isotope ratio without unit.

15. The following expressions are applicable to convert activity to concentration; for uranium-238 and thorium-232:
1 ppm U=12.4 Bq/kg238U, 1 ppm Th=3.93 Bq/kg232Th.

16. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:
δyI=1,000×(Ksample-Kstandard)/Kstandard, where K= the isotope ratio and yI =2H, 18O, 37Cl, 13C or 34S etc.

17. SKB estimation from duplicate analyses by the contracted laboratory.

# Appendix 2

## Corrected borehole section information

| ID code | Sample no. | Elevation (m.a.s.l.) | Corrected values | | | Original Values | | |
|---|---|---|---|---|---|---|---|---|
| | | | Secup | Secmid | Seclow | Secup | Secmid | Seclow |
| DA1619A02 | 20406 | | 0.00 | 47.00 | 94.45 | | | |
| HA1330B | 3465 | –183.13 | 6.00 | 19.25 | 32.50 | 0.00 | 16.25 | 32.50 |
| KA2511A | 6760 | –404.41 | 111.00 | 124.50 | 138.00 | 187.00 | 188.50 | 190.00 |
| KA2563A | 6761 | –466.54 | 187.00 | 188.50 | 190.00 | 111.00 | 124.50 | 138.00 |
| | 2437 | | 187.00 | 191.50 | 196.00 | 187.00 | 191.50 | 196.00 |
| KA3065A03 | 6918 | –408.89 | 10.74 | 11.00 | 11.23 | 10.72 | 11.00 | 11.28 |
| KA3539G | 2594 | –463.96 | 0.00 | 15.01 | 30.01 | 15.00 | 16.50 | 18.00 |
| | 14023 | –465.66 | 15.85 | 16.73 | 17.60 | | | |
| KA3548A01 | 14024 | –447.08 | 8.80 | 9.78 | 10.75 | 0.00 | 15.00 | 30.00 |
| KA3554G01 | 14022 | –465.34 | 22.60 | 23.38 | 24.15 | 0.00 | 15.01 | 30.01 |
| KA3573A | 2619 | –447.11 | 18.00 | 29.04 | 40.07 | 18.00 | 29.00 | 40.00 |
| KA3590G01 | 6211 | | 7.00 | 11.00 | 15.00 | 15.20 | 19.35 | 23.50 |
| | 6265 | | | | | | | |
| | 6936 | | 16.00 | 23.03 | 30.06 | 12.20 | 17.85 | 23.50 |
| | 14029 | | 7.00 | 11.00 | 15.00 | | | |
| KA3593G | 2570 | –462.82 | 0.00 | 15.01 | 30.02 | 0.00 | 15.00 | 30.00 |
| KA3600F | 6268 | –446.78 | 40.50 | 41.25 | 42.00 | 0.00 | 25.05 | 50.10 |
| | 14025 | | | | | | | |
| | 3807 | –446.94 | 43.00 | 46.55 | 50.10 | 4.50 | 12.75 | 21.00 |
| | 3808 | –446.78 | 40.50 | 41.25 | 42.00 | 22.00 | 36.00 | 50.01 |
| KJ0044F01 | 2832 | –447.76 | 1.00 | 9.13 | 17.26 | 0.00 | 8.63 | 17.26 |
| | 3764 | | | | | | | |
| | 6220 | | | | | | | |
| | 6706 | | | | | | | |
| | 14447 | | | | | | | |
| | 14592 | | | | | | | |
| | 3154 | | | | | 16.00 | 16.63 | 17.26 |
| KR0012B | 6364 | –69.12 | 4.00 | 7.29 | 10.57 | 0.00 | 5.29 | 10.57 |
| | 6745 | | | | | | | |
| | 3826 | –69.16 | | | | 5.00 | 7.79 | 10.57 |
| KR0013B | 6360 | –69.23 | 6.00 | 11.47 | 16.94 | 0.00 | 8.47 | 16.94 |
| | 3445 | –69.23 | | | | 1.20 | 9.05 | 16.90 |
| | 3818 | –69.24 | | | | 7.05 | 12.00 | 16.94 |
| KR0015B | 6361 | | 18.80 | 24.55 | 30.31 | 0.00 | 15.15 | 30.31 |
| | 3446 | –69.35 | 1.20 | 15.75 | 30.31 | 1.20 | 15.75 | 30.30 |
| | 6182 | | 18.80 | 24.55 | 30.31 | 18.80 | 24.55 | 30.31 |
| | 6990 | | | | | | | |
| | 14395 | | | | | | | |
| | 14596 | | | | | | | |
| | 14923 | | | | | | | |
| | 20397 | | | | | | | |
| | 20734 | | | | | | | |
| | 20996 | | | | | | | |
| | 3819 | | | | | 19.82 | 25.06 | 30.31 |

| ID code | Sample no. | Elevation (m.a.s.l.) | Corrected values | | | Original Values | | |
|---|---|---|---|---|---|---|---|---|
| | | | Secup | Secmid | Seclow | Secup | Secmid | Seclow |
| SA1420A | 6963 | –200.56 | 6.00 | 28.00 | 50.00 | 0.00 | 25.00 | 50.00 |
| | 14392 | | | | | | | |
| | 14597 | | | | | | | |
| | 6712 | | | | | 1.00 | 25.50 | 50.00 |
| SA1730A | 3332 | –236.98 | 5.60 | 12.80 | 20.00 | 6.00 | 13.00 | 20.00 |
| | 3458 | | | | | | | |
| SA2273A | 3336 | –305.94 | 5.80 | 12.90 | 20.00 | 6.00 | 13.00 | 20.00 |
| | 3470 | | | | | | | |
| SA2600A | 3450 | –345.02 | 5.80 | 12.60 | 19.40 | 0.00 | 9.70 | 19.40 |
| | 3337 | | | | | 6.00 | 12.70 | 19.40 |
| SA2783A | 3345 | –371.33 | 5.80 | 12.85 | 19.90 | 6.00 | 12.95 | 19.90 |
| SA2880A | 14008 | –384.71 | 6.00 | 12.95 | 19.90 | 0.00 | 9.95 | 19.90 |
| | 14451 | | | | | | | |
| | 3344 | | | | | 6.00 | 12.75 | 19.50 |
| | 2338 | | | | | 11.92 | 12.92 | 13.92 |
| | 2384 | | | | | | | |
| | 2449 | | | | | | | |
| | 2505 | | | | | | | |
| | 2651 | | | | | | | |
| | 2906 | | | | | | | |
| | 2989 | | | | | | | |

# Appendix 3

## Plotted Eh and pH measurement sequences

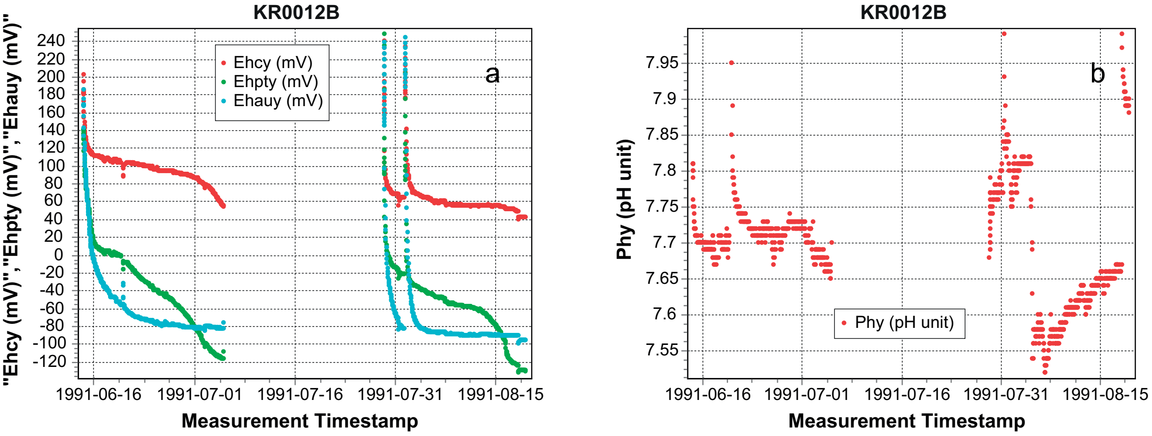

*Figure A3-1 a, b. Redox project, borehole KR0012B section 5.04–10.57 m, secmid elevation –69.17 m, a) Eh versus date, selected Eh= –110 mV and b) pH versus date, selected pH=7.7.*

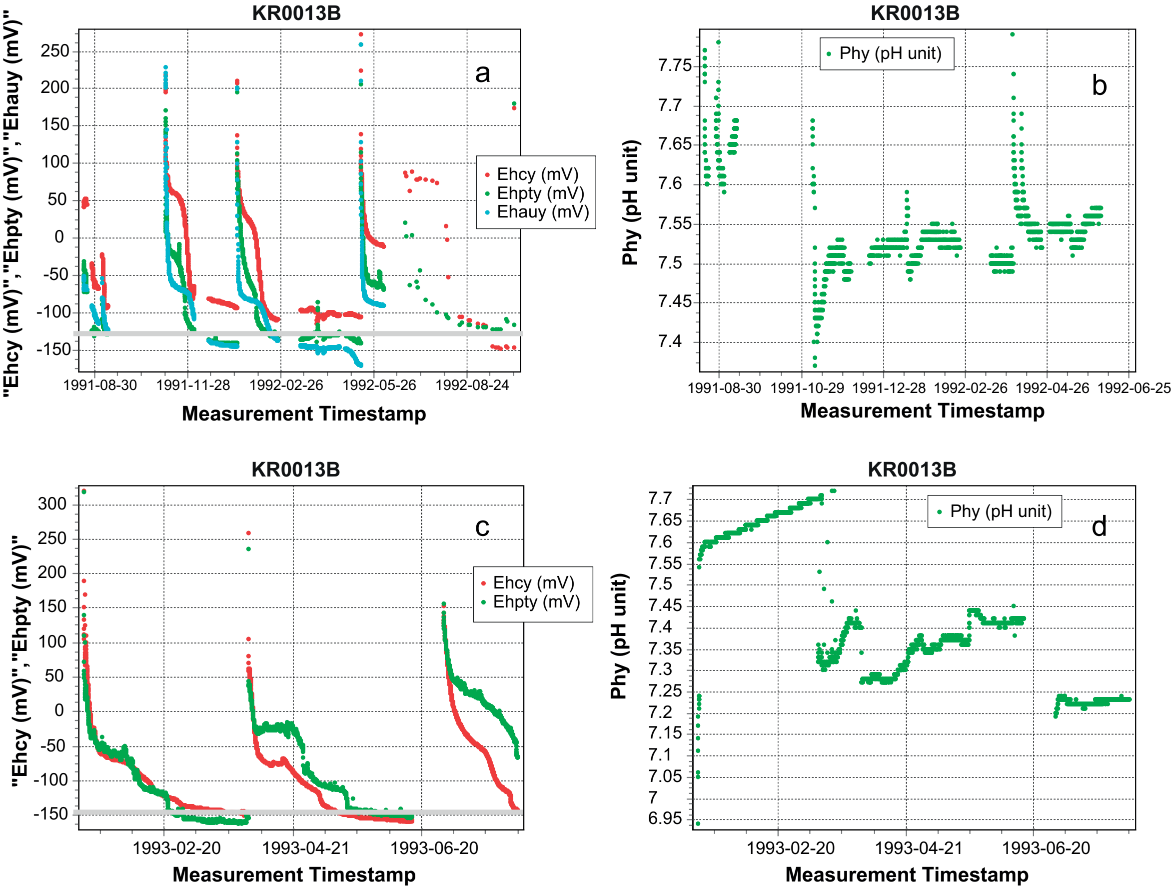

*Figure A3-2 a–d. Redox project, borehole KR0013B section 7.00–26.94 m, secmid elevation –69.2 m, a) Eh versus date, selected Eh=–130 mV, b) pH versus date, selected pH=7.5. Repeated measurements, c) selected Eh=–150 mV and d) selected pH=7.35.*

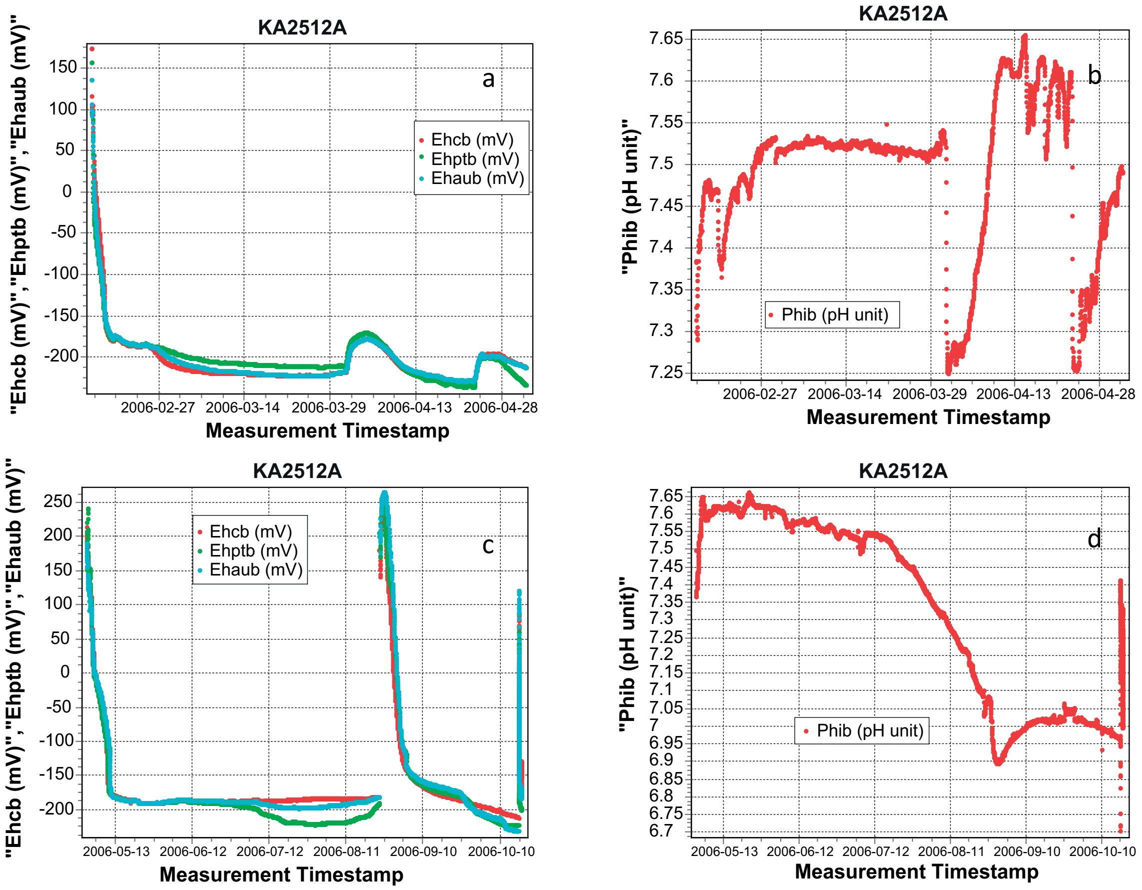

***Figure A3-3 a–d.*** *Prototype project, borehole KA2512A section 0–37.27 m, elevation –336.4 m. a) Eh versus date, selected Eh=–221 mV, b) pH versus date, selected pH 7.5. Repeated measurements, c) selected Eh=–200 mV and d) Selected pH=7.6.*

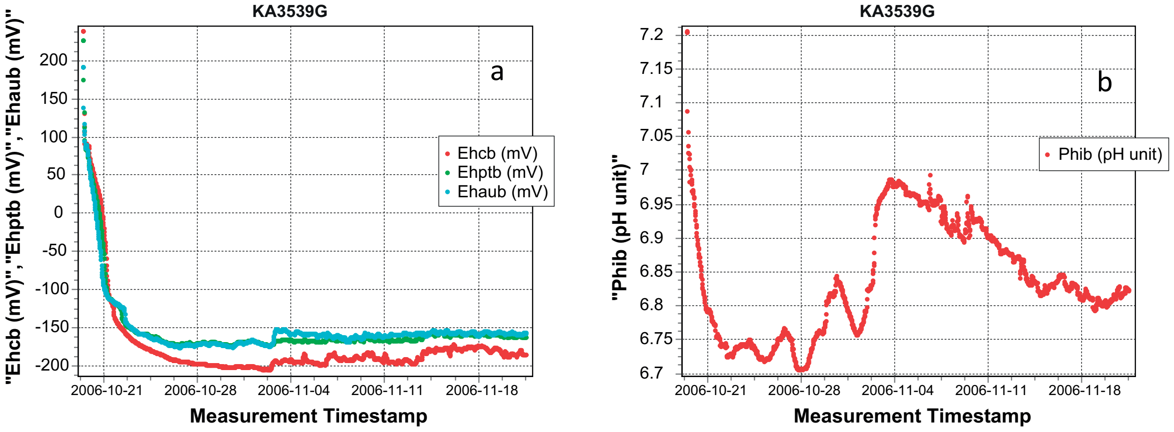

***Figure A3-4 a, b.*** *Prototype project, borehole KA3539G section 15.85–17.60 m, elevation –465.73 m, a) Eh versus date, selected Eh=–170 mV and b) pH versus date, selected pH=6.8.*

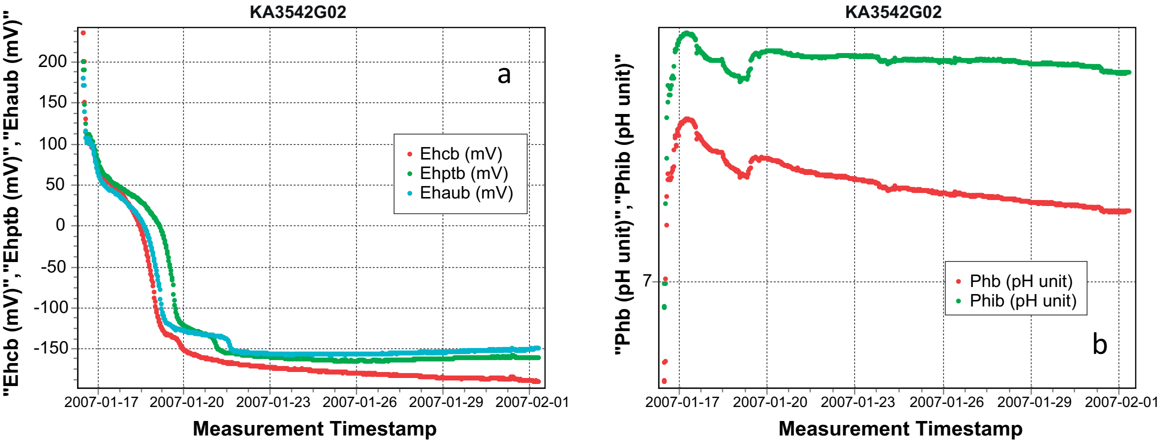

***Figure A3-5 a, b.*** *Prototype project, borehole KA3542G02 section 25.6–27.2 m, elevation –467.17 m, a) Eh versus date, selected Eh=–167 mV and b) pH versus date, selected pH=7.4.*

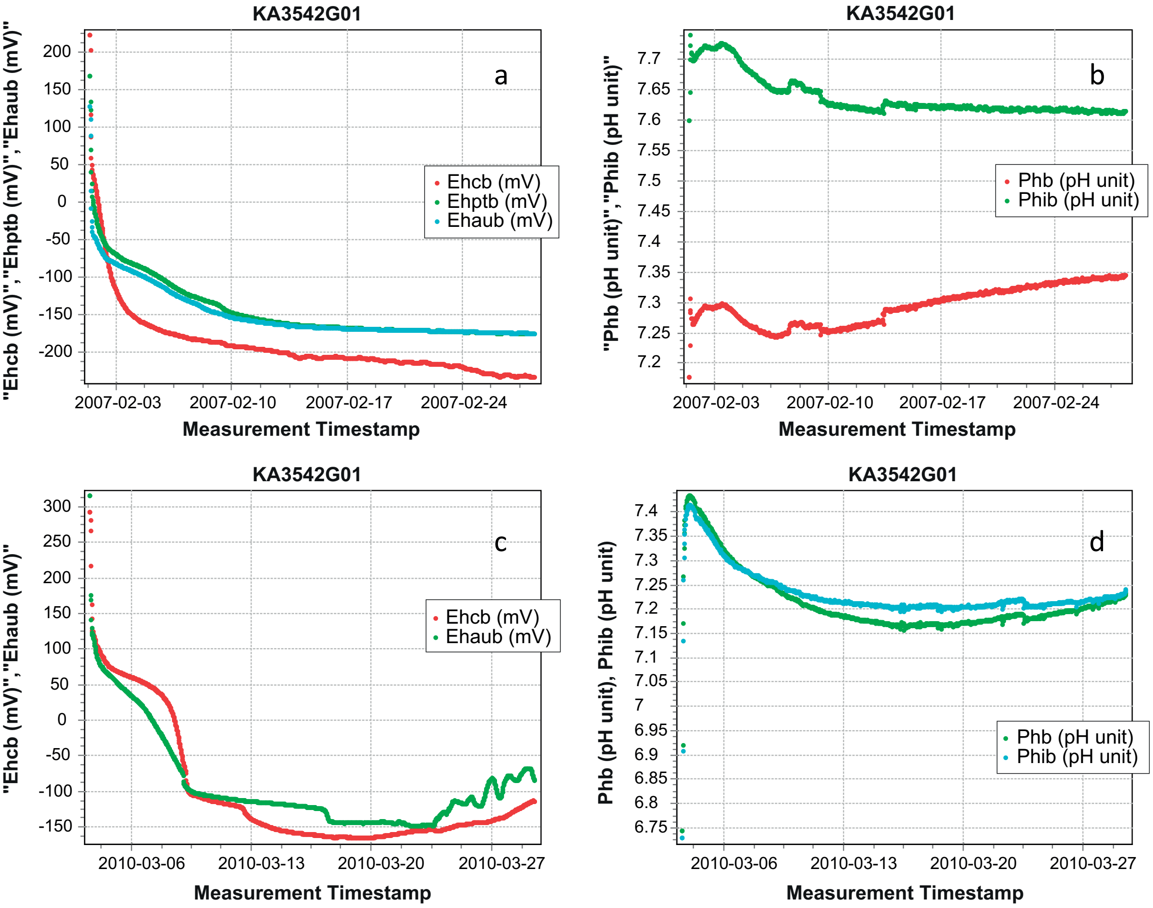

***Figure A3-6 a–d.*** *Prototype project, borehole KA3542G01 section 16.6–20.3 m, elevation –462.78 m, a) Eh versus date, selected Eh=–196 mV and b) pH versus date, selected pH=7.5. Repeated measurements, c) selected Eh=–153 mV and d) selected pH= 7.2.*

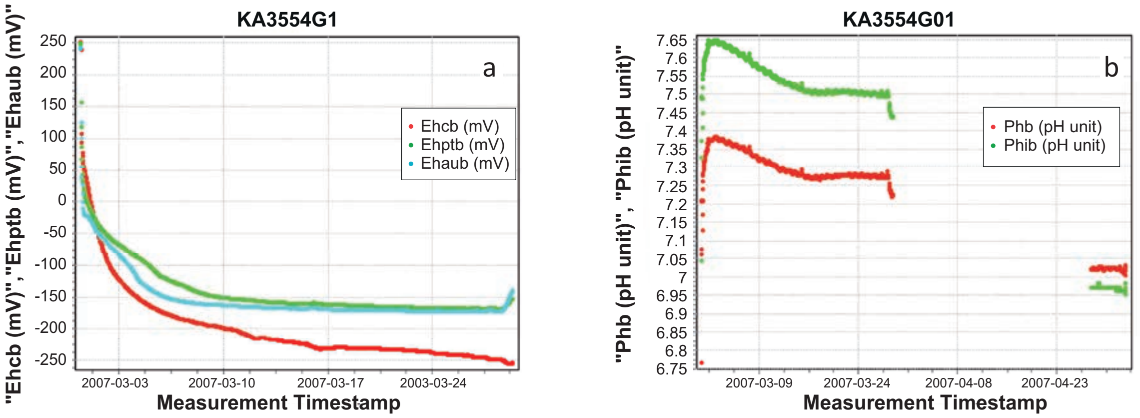

***Figure A3-7 a, b.*** *Prototype project, borehole KA3554G01 section 22.6–24.2 m, elevation –465.39 m, a) Eh versus date, selected Eh=–183 mV and b) pH versus date, selected pH=7.3.*

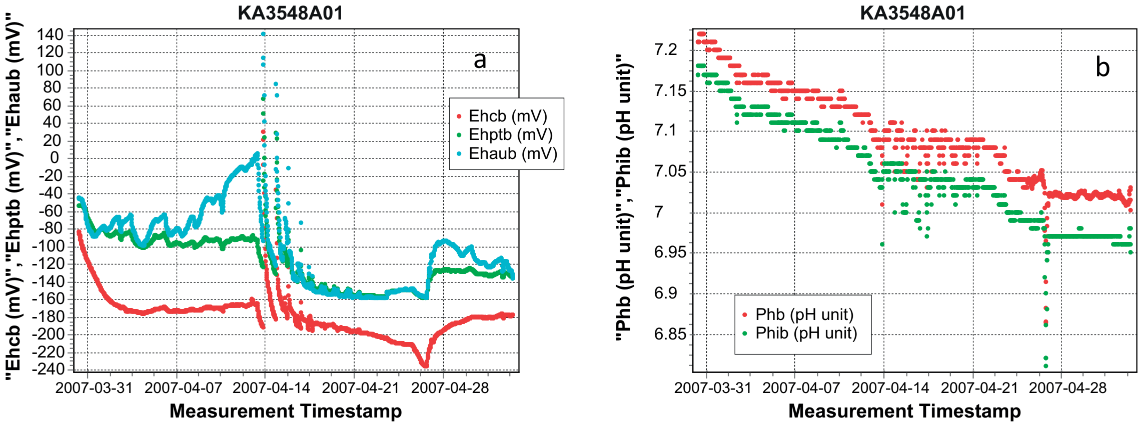

***Figure A3-8 a, b.*** *Prototype project, borehole KA3548A01 section 8.8–10.8 m, elevation –447.11 m, a) Eh versus date, selected Eh=–170 mV and b) pH versus date, selected pH= 7.0.*

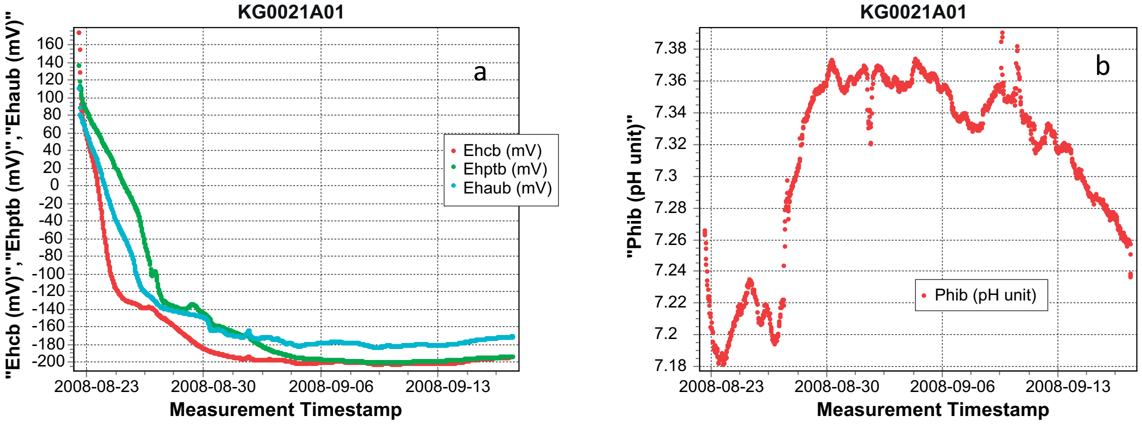

***Figure A3-9 a, b.*** *Prototype project, borehole KG0021A01 section 35.0–36.0 m, elevation –434.38 m, a) Eh versus date, selected Eh=–187 mV and b) pH versus date, selected pH=7.24.*

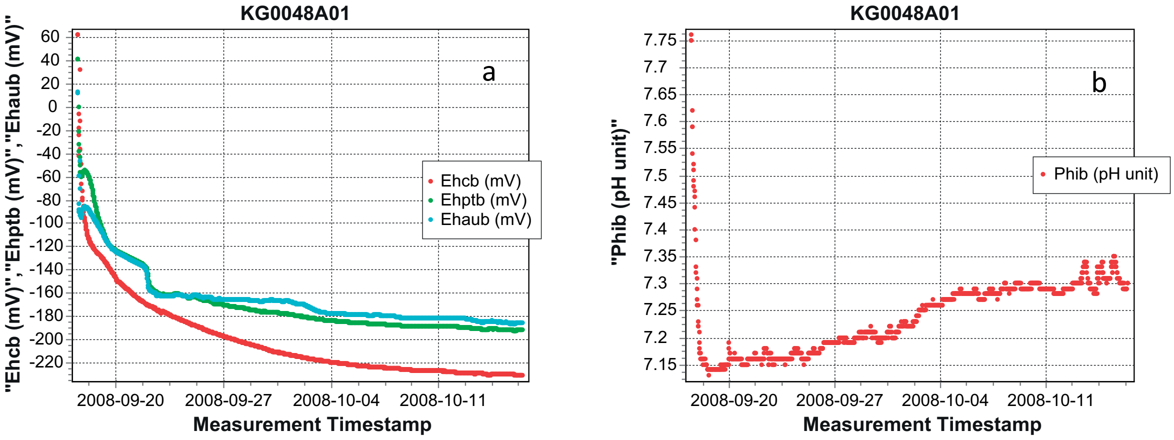

***Figure A3-10 a, b.*** *Prototype project, borehole KG0048A01 section 32.8–33.8 m, elevation –436.43 m. a) Eh versus date, selected Eh=–203 mV and b) pH versus date, selected pH=7.3.*

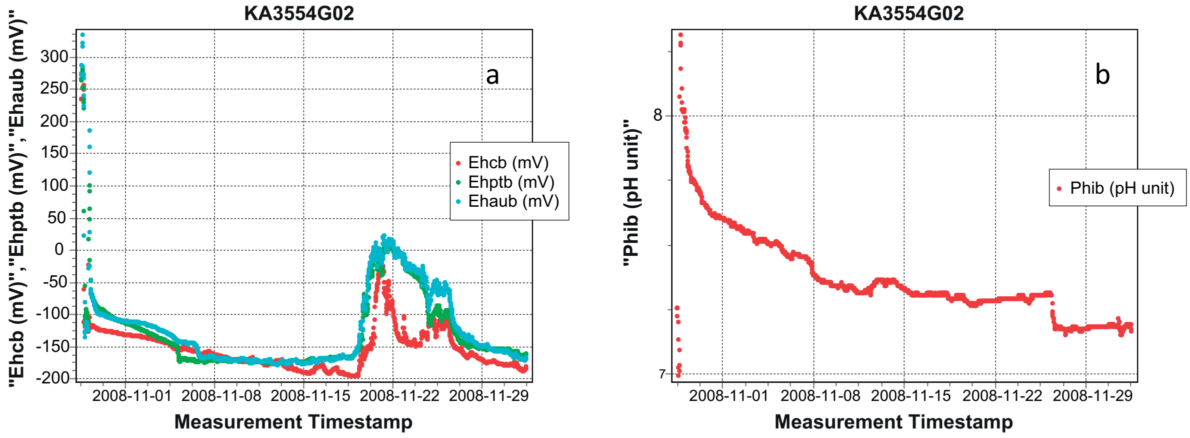

***Figure A3-11 a, b.*** *Prototype project, borehole KA3554G02 section 10.5–12.2 m, elevation –456.84 m a) Eh versus date, selected Eh=–170 mV and b) pH versus date, selected pH=7.2.*

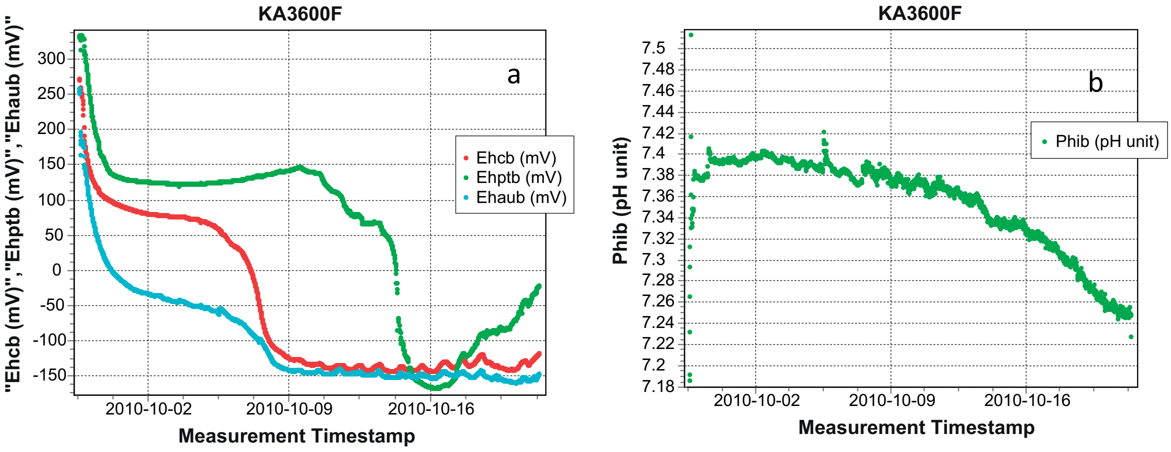

***Figure A3-12 a, b.*** *Prototype project, borehole KA3600F section 40.5–42.0 m, elevation –446.8 m, a) Eh versus date, selected Eh=–150 mV and b) pH versus date, selected pH=7.34.*