

Forsmark site investigation

Chemical characterisation in borehole KFM07A

Results from the investigated section at 848.0–1001.6 m

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September 2005

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors and do not necessarily coincide with those of the client.

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Abstract

Complete chemical characterisation is the most extensive chemical investigation method performed in core drilled boreholes. The method entails pumping, measurements on-line and regular water sampling for chemical analyses in isolated borehole sections. This is carried out over a period of approximately three weeks per section at a flow rate of between 50 and 200 mL/min.

The method has been used in a section from borehole KFM07A at 848.0–1,001.6 m borehole length. In reality a water bearing fracture zone was identified at approximately 970 m, but due to blocking out-falls from the borehole wall below 850 m, it was necessary to create a long section for groundwater sampling delimited by a single packer and the bottom of the borehole.

The results obtained from the complete chemical characterisation of section 848.0–1,001.6 include on-line measurements of redox potential, pH, dissolved oxygen, electrical conductivity and water temperature in the borehole section as well as chemical analyses of major constituents, trace metals and isotopes. Furthermore, gas content and composition, inorganic colloids as well as humic and fulvic acids were investigated.

The water composition was stable during the pumping and sampling period. The chloride concentration amounted to 14,800 mg/L, i.e. the highest value obtained so far at the Forsmark site. Due to heavy pumping during and after drilling, the borehole was filled to the groundwater table with this saline water which might have originated from even larger depths than 840 m (corresponding to fracture zone at 970 m borehole length). The measured redox potential of approximately + 9 mV is not a plausible value at this depth and the result is difficult to explain. However, considering that deep saline water has been temporarily forced to ascend all the way to the groundwater table, it can not be completely excluded that these circumstances have affected the redox conditions. The content of inorganic colloids was low and the organic constituents were present mainly as fulvic acids or other low molecular weight acids (citric acid, oxalic acids, etc).

Sammanfattning

Fullständig kemikaraktärisering är den mest omfattande kemiska undersökningsmetoden för kärnbron. Metoden innebär pumpning, mätning on-line och regelbunden vattenprovtagning för kemiska analyser i avgränsade bronsektioner under cirka tre veckor per sektion med ett pumpflöde på mellan 50 och 200 mL/min.

Metoden har utförts i en sektion av bron KFM07A vid 848.0–1 001.6 m bronslängd. En vattenförande sprickzon identifierades vid cirka 970 m. På grund av blockering av utfall från bronsvägg vid ca 850 m var det nödvändigt att skapa en lång sektion som begränsades av en övre manschett och bronns botten.

Resultaten som erhöles från den fullständiga kemikaraktäriseringen av sektionen 848.0–1 001.6 m omfattar mätningar on-line av redoxpotential, pH, löst syre, elektrisk konduktivitet och vattentemperatur i bronsektionen, liksom kemiska analyser av huvudkomponenter, spårelement och isotoper. Vidare undersöktes gasinnehåll och sammansättning, oorganiska kolloider samt humus- och fulvosyror i grundvattnet.

Vattensammansättningen var stabil under pump/provtagningsperioden. Kloridkoncentrationen uppgick till ca 14 800 mg/L vilket är den högsta koncentration som uppmätts hittills i Forsmarksområdet. På grund av kraftig pumpning under och efter bronningen fylldes hela bron med detta salta vatten, som kan härröra från ännu större djup än 840 m (motsvarande sprickzonen vid 970 m bronslängd). Redoxpotentialen uppgick till cirka + 9 mV vilket inte är ett rimligt värde på detta djup och resultatet är svårt att förklara. En situation där djupt och salt vatten tillfälligt lyfts hela vägen till ytan är dock ovanlig och det kan inte helt uteslutas att dessa omständigheter har påverkat redoxförhållandena. Innehållet av oorganiska kolloider var lågt och de organiska komponenterna förelåg huvudsakligen som fulvosyror eller andra lågmolekylära syror (citronsyra, oxalsyra etc).

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1 Introduction

This document reports performance and results of the activity Complete chemical characterisation in KFM07A within the site investigation programme at Forsmark /1/. The work was conducted according to the activity plan AP PF 400-05-012. The report presents hydrogeochemical data from the borehole section at 848.0–1,001.6 m resulting from fieldwork carried out during March and April 2005. The controlling documents for this activity are listed in Table 1-1. Both activity plan and method description are SKB's internal controlling documents. The obtained data from the activity are reported in the database SICADA and traceable by the activity plan number. Sampling for microbe studies, based on the activity plan AP PF 400-05-66 (SKB internal controlling document) was likewise performed within the present activity. The microbe investigations are reported in a separate primary data report /2/.

Borehole KFM07A is the seventh approx 1,000 m deep telescopic borehole drilled at Forsmark /3/. The location of the borehole and the other current deep telescopic boreholes within the investigation area are shown in Figure 1-1, whereas Figure 1-2 presents a detailed map of drill site DS7 with KFM07A and nearby situated percussion drilled boreholes in rock and soil. KFM07A is inclined at 60°, dipping west. However, the borehole deviates slightly towards northwest versus depth. The borehole section between 0–100.40 m is percussion drilled and has a stainless steel casing with an internal diameter of 200 mm. Section 100.40–101.70 m is core drilled with a diameter of 86.0 mm and cased. Finally, section 101.70–1,001.55 m is core drilled with a diameter 77.3 mm and uncased. The design of the borehole is presented in Appendix 1.

The borehole is of the so-called SKB chemical-type; see the SKB method descriptions MD 620.003 (Method description for drilling cored boreholes) and MD 610.003 (Method description for percussion drilling). An SKB chemical-type borehole requires cleaning procedures to be carried out on all equipment to be used in the borehole, both during and after drilling, according to level 2 in the cleaning instructions outlined in MD 600.004 (Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning). The method descriptions and instructions are SKB internal controlling documents.

Table 1-1. Controlling documents for performance of the activity.

Activity plan	Number	Version
Fullständig kemikaraktärisering med mobilt fältlaboratorium i KFM07A.	AP PF 400-05-012	1.0
Method descriptions	Number	Version
Metodbeskrivning för fullständig kemikaraktärisering med mobilt fältlaboratorium.	SKB MD 430.017	1.0

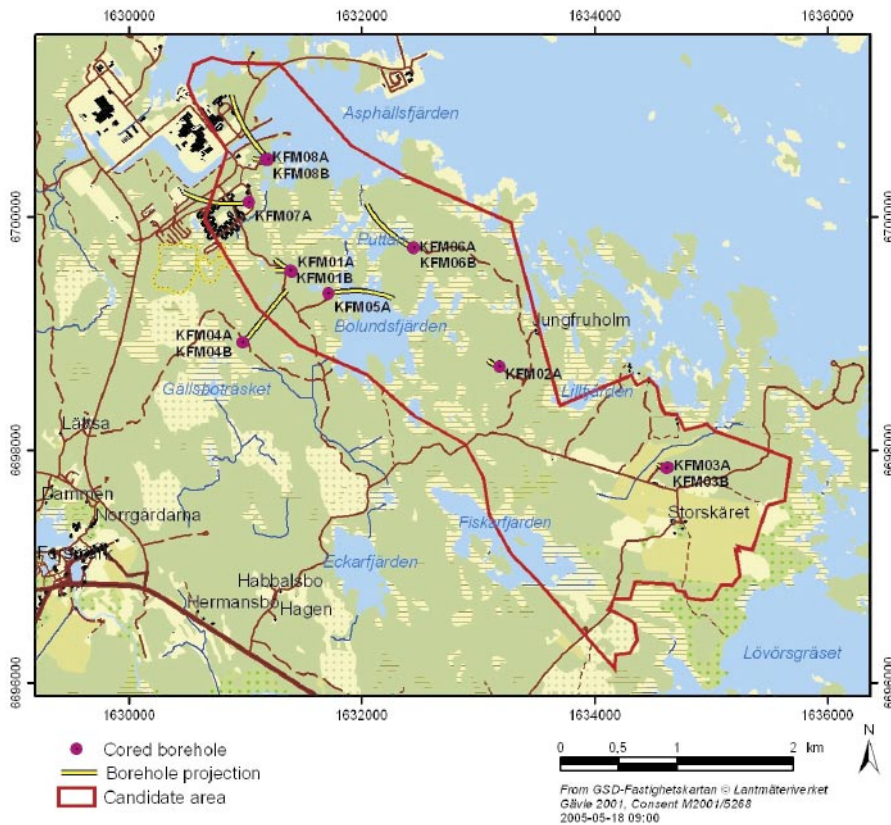


Figure 1-1. The investigation area at Forsmark (approximately the area inside the black square) including the candidate area selected for more detailed investigations. The deep and semi deep (approx. 100–450 m) cored boreholes, KFM01A to KFM08B, are marked with pink infilled circles.

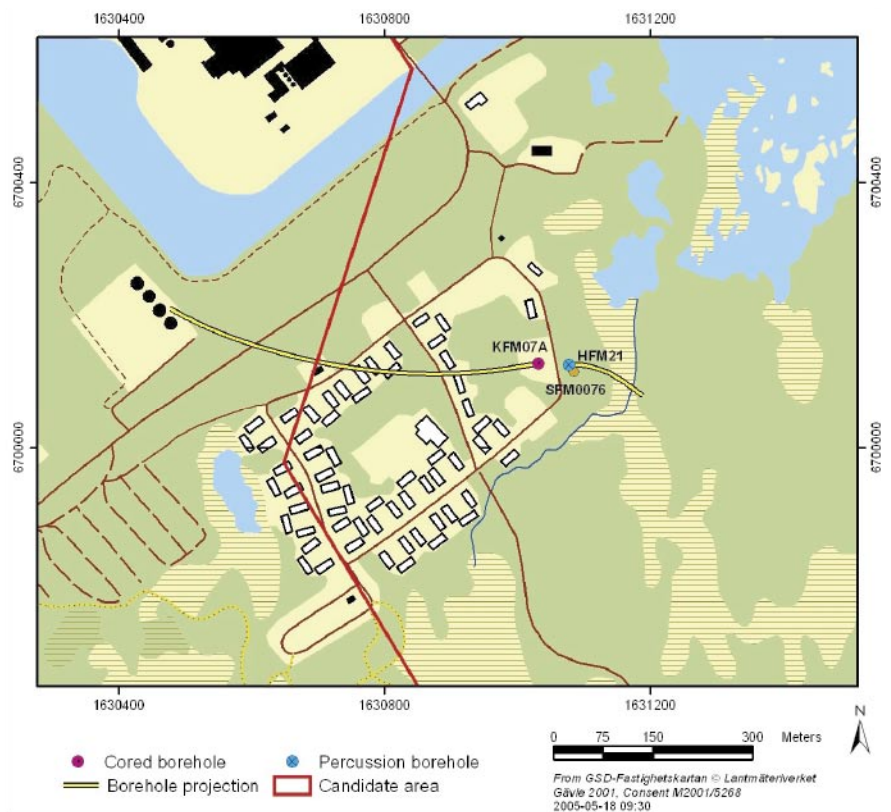


Figure 1-2. Location and projection on the horizontal plane of the cored borehole KFM07A, the percussion borehole HFM21 and the shallow monitoring well in soil SFM0076 at drill site DS7.

2 Objectives and scope

Complete chemical characterisation is the most extensive chemical investigation method performed in core drilled boreholes. The method is carried out in order to get as much information as possible about the groundwater chemical conditions in individual water bearing fractures or local minor fracture zones. Considerable effort is put into obtaining representative samples from a limited rock volume. Careful pumping and continuous control of the pressure in the sampled borehole section, as well as above the section, is maintained in order to minimise the risk of mixing with water from other fracture systems.

A decision has been made to prioritise the northwestern part of the Forsmark candidate area for continuing investigations /4/. So far, representative chemical data from borehole sections at depths greater than 200 m have been scarce from this part of the area. Besides the section at 848.0 to 1,001.6 m presented here, the only other deeper sections investigated have been at approx 307 m and 700 m depths in KFM06A. Furthermore, there are reasons to believe that there will be very few water yielding fractures at depth also in the coming boreholes. Therefore, every opportunity to conduct chemical investigations at depth, in this part of the candidate area, needs to be taken.

The analytical programme was carried out according to SKB chemistry class 4 and class 5 including all options. Furthermore, pH, redox potential (Eh) and water temperature were measured in flow-through cells downhole in the borehole as well as at the ground surface. The flow-through cell at the surface also measured electrical conductivity and dissolved oxygen. Samples were collected in situ in the borehole section for determination of gas content and composition, microbe content and their characterisation as well as for colloid investigation. Fractionation of organic acids and inorganic species were performed to investigate size distribution (DOC and ICP analyses). Enrichment of organic acids was conducted in order to allow determination of $\delta^{13}\text{C}$ and pmC in organic constituents.

3 Background

3.1 Flushing water history

The percussion drilled borehole HFM21 served as a supply well for the flushing water, used to drill borehole KFM07A /5/. The chemical composition of the flushing water was checked before and during use. The hydrochemical data from the supply well HFM21 are reported in /6/. The core drilling of the 1,000 m long borehole consumed 1,121 m³ of flushing water and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 2,300 m³. The nominal concentration of the dye Uranine, added as a tracer to mark the flushing water, was 0.2 mg/L. Automatic dosing equipment to introduce Uranine was installed in the flushing water line to supply flushing water to the drilling. The Uranine concentration in the flushing water and return water was checked regularly during drilling by the drilling crew and a total of 116 and 120 samples, respectively, were analysed as an immediate test of the dosing system and the recovery of flushing water. A selected set of 30 flushing water and 23 return water samples were also analysed by laboratory personnel in the field laboratory. The laboratory results were found more reliable and are therefore used in further evaluations. The average Uranine concentration (laboratory analyses) in the flushing water pumped into the borehole was 0.213 ± 0.016 mg/L. The laboratory values are presented in Figure 3-1 and used in the budget calculations in Table 3-1, where the amount of Uranine added to the borehole via the flushing water and the estimated amount recovered in the return water are given.

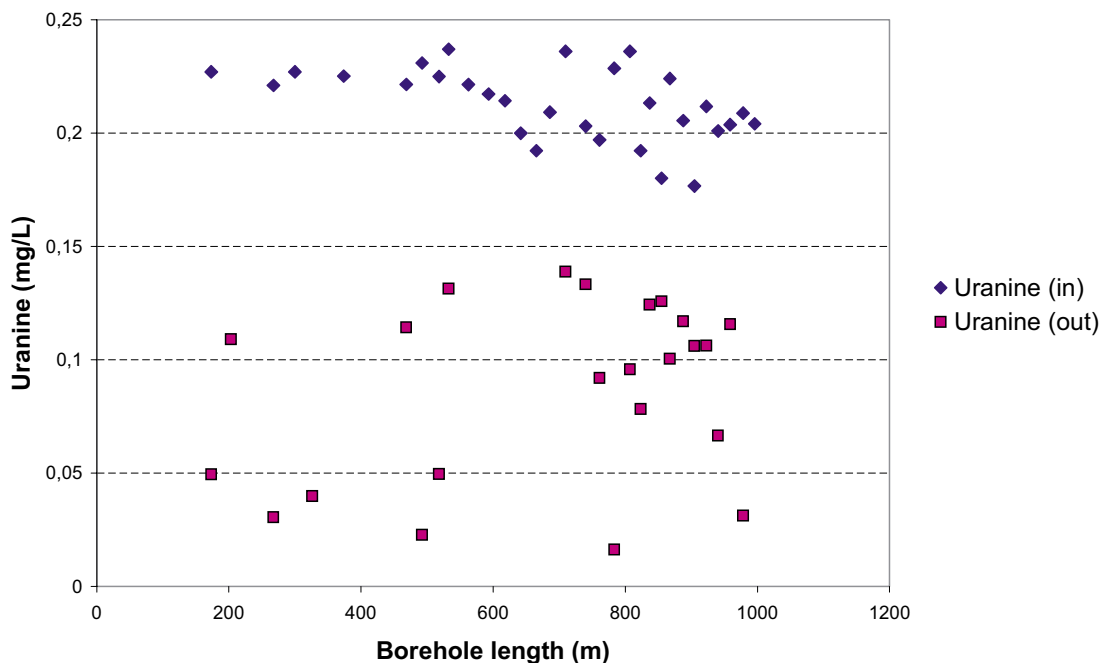


Figure 3-1. Uranine concentrations in the flushing water and in the return water versus borehole length. The addition of Uranine was carried out using the automatic dosing equipment which is controlled by a flow meter.

Table 3-1. Amount of Uranine added to KFM07A via the flushing water during core drilling and the amount recovered from the contemporary air-lift pumping.

Uranine	(g)
Added, according to the log book.	255
Added, calculated from the average Uranine concentration (lab) and the total volume of flushing water.	239
Recovered, estimated from the average Uranine concentration (lab) and the total volume of return water.	181

The Uranine budget in Table 3-1 suggests that between 300 and 370 m³ of the flushing water was lost to the borehole and the adjacent host bedrock. After the completed drilling, the pumping was continued and an additional volume of 1,476 m³ was pumped out but no Uranine analyses were performed on that volume.

As borehole KFM07A is of SKB chemical-type, the following special precautions were taken in order to minimise contamination via the flushing water:

- The supply well was also of SKB chemical-type.
- Borehole HFM21 was selected to supply flushing water because of the low concentration of total organic carbon (TOC). The concentration should preferably be below 5 mg/L, and the concentration in the samples collected in HFM21 was in the range 3.9–5.0 mg/L.
- Dosing equipment for Uranine was installed, thereby removing the need for an in-line flushing water storage tank after the UV-system. Using a storage tank involves a potential risk of bacterial growth.

The microbe content in the flushing water was not determined during drilling of this borehole. The microbe results from drilling of the preceding borehole KFM06A /7/ showed convincingly that the cleaning procedure works well. It was therefore concluded that check of microbes at all drilling occasions was no longer necessary.

3.2 Previous events and activities in the borehole

KFM07A is an SKB chemical-type core borehole and thus specially intended for complete hydrochemical characterisation. Only those investigations that are necessary in order to select borehole sections are carried out in the borehole prior to the chemistry campaign. The more down-hole equipment used in the borehole, the greater is the risk of contamination and effects on the in situ microbiological conditions. However, due to a tight time schedule, one exception was made in KFM07A, and injection tests were allowed to precede the chemical investigation. The activities/ investigations performed in KFM07A prior to the chemistry campaign are listed in Table 3-2 below.

Table 3-2. Activities performed in KFM07A prior to the chemical characterisation.

Activities performed	Date of completion	Length or section (m)	Comment
Percussion drilling	2004-06-16	0–100.40	
Wire-line water sampling class 3	2004-10-28	100.4–305.84	Sample no 8712
Core drilling	2004-12-09	100.40–1,001.55	HFM21 was the source of flushing water for drilling the cored part of KFM07A. HFM21 is an SKB chemical-type borehole /3, 5/. Flushing water volume = 1,121 m ³ , Return water volume 2,300 m ³ .
Clean-up pumping	2004-12-23 to 2005-01-05		Pumped volume = 1,476 m ³ .
Flushing water treatment	–	–	Automatic dosing of Uranine was used during drilling of KFM07A. In this way no in-line storage tank was needed after the UV-system /3/.
Microbe control of flushing water was not performed	–	–	–
BIPS-logging	2005-01-11	101–950	/8/
Radar logging	2005-01-14	100–ca 990	Maximum investigated borehole length varies at different occasions.
Differential flow logging	2005-01-29	0–ca 900	The equipment was lowered to different depths each time and did not reach the bottom at all occasions. The reason was problems with rock out-falls in the borehole /9/. The logging revealed that the entire borehole was filled with saline water from depth.
BIPS-logging	2005-02-09	550–993	/8/
Geophysical logging	2005-02-09	102–ca 993	/10/
Injection tests	2005-03-01	104–1,001.55	Due to logistic advantages, the injection tests were performed before chemical characterisation /11/.
Hydrochemical logging	2005-03-09	0–995	Sample nos 8810 to 8824 /12/. The results verified that the water column along the borehole consisted of very saline water emerging from depth. However, the saline front had descended to a somewhat deeper level with time.
Hydrochemical characterisation	2005-04-07	848–1,001.55	Presented in this report.
Microbe investigation	2005-04-07	848–1,001.55	/2/

3.3 Choice of borehole sections

The differential flow logging prior to the chemical investigation revealed one water bearing fracture in the deep part of the borehole at approximately 970 m. However, since the lowering of the flow logging equipment below 856 m borehole length succeeded only once (the first occasion and without pumping) due to out-fall from the borehole wall, therefore, the water yield was uncertain. Furthermore, several water bearing fractures/fracture zones were revealed between 100 m and 261 m borehole length. The fractures/fracture zones with a water yield large enough to allow water sampling (hydraulic transmissivity $\geq 10E-8$ m²/s) are listed in Table 3-3.

Due to lack of deep data from this part of the candidate area, selection of the probable zone at 970 m was obvious. The more shallow depths were regarded as less important to investigate and were therefore excluded. Rock out-fall in the borehole prevented the downhole equipment from reaching the planned depth, this made it necessary to create a long section delimited by one packer at 848 m and the bottom of the borehole. Section limits and the corresponding hydraulic transmissivity value for the resulting section are given in Table 3-4.

The differential flow log for this part of the borehole is given in Appendix 2 and the corresponding image from the BIPS-logging (Borehole Image Processing System) is presented in Appendix 3.

Table 3-3. Water yielding fractures/fracture zones identified from differential flow logging of KFM07A, determined flow rates and flow directions (approximately 10 m drawdown). The selected fracture is given in bold text.

Borehole length (m)	Flow (L/h)	Flow direction (in or out from borehole)	Comments
110–113	> 200	In	Several fractures
116–117	20	In	
119–123	> 200	In	Several fractures
133.7	> 200	Out	
143.8	80	Out	
178.5	> 200	In	
261.4	a few litres	Out	
970.0	uncertain	–	Approx 2 L/h without pumping

Table 3-4. Selected borehole section and hydraulic transmissivity value calculated from differential flow logging (T_D) and from injection test (T_I).

Section (m)	Differential flow logging, T_D /9/ (m ² /s)	Injection tests, T_I (m ² /s) /11/	Comments
848.00–1,001.55	See comments.	9.7×10^{-8}	Differential flow logging during pumping was not performed below circa 891 m. Thus, the transmissivity of deeper fractures/fracture zones could not be determined. Differential flow logging under natural (unpumped) conditions indicates small fractures at approx 916 and 917 m and a larger fracture at 970.0 m. Injection tests: Due to a cavity in the borehole at approx 860 m, only a single-packer injection test was made below 850 m.

4 Equipment

4.1 The mobile field laboratory (MFL)

The mobile field laboratories used by SKB for water sampling and downhole measurements consist of a laboratory unit, a hose unit with downhole equipment and a Chemmac measurement system; the system is presented schematically in Figure 4-1. It is also possible to include a separate unit for computer work (MYC). The different parts of the system are described in the SKB internal controlling documents SKB MD 434.004, 434.005, 434.006, 434.007 and SKB MD 433.018 (Mätssystembeskrivningar för mobil kemienhet allmän del, slangvagn, borrhålsutrustning, mobil ytChemmac och dataapplikation).

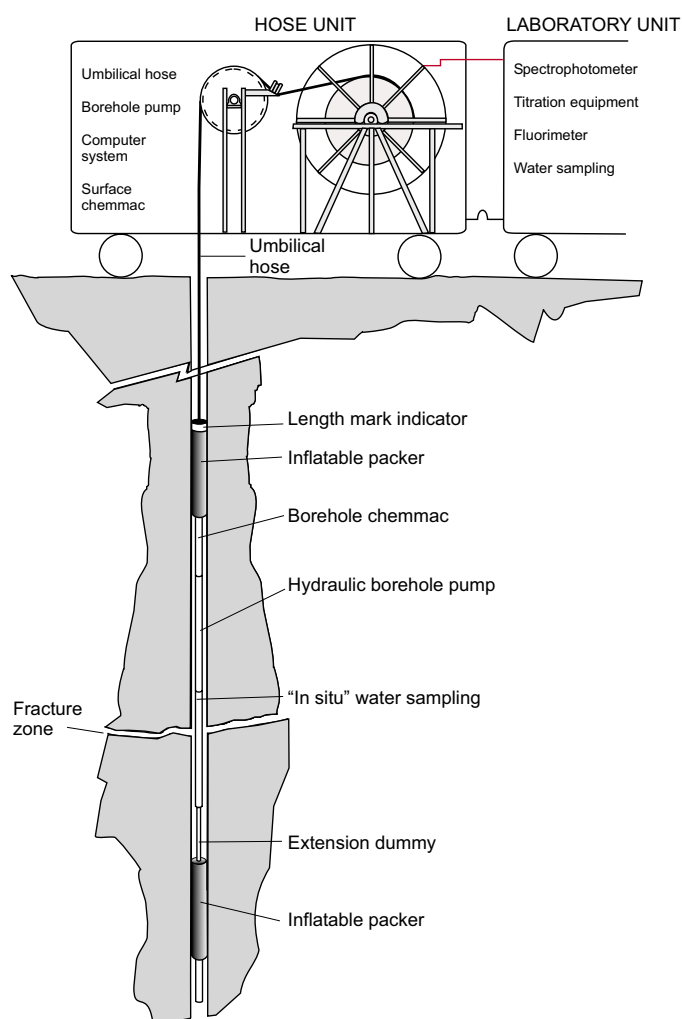


Figure 4-1. The mobile laboratory including laboratory unit, hose unit and downhole equipment. The configuration of the downhole units in the borehole can be varied depending on desired section length. However, the in situ water sampler must always be positioned first in the sample water path. In this particular case, a single packer was used with the bottom of the borehole constituting the lower section limit.

The Chemmac measurement facilities include communication system, measurement application and flow-through cells with electrodes and sensors at the ground surface (surface Chemmac) and downhole (borehole Chemmac).

The downhole equipment comprises of inflatable packers, pump, borehole Chemmac and the in situ sampling unit (PVP), allowing measurement (borehole Chemmac) and sampling in situ in the borehole section (PVP sampling unit). The four sample portions collected with the PVP sampling unit maintain the pressure from the borehole section when raised to the surface. The portions are used for colloid filtration, gas analyses and microbe investigations.

The mobile units used for the investigation of borehole KFM07A consisted of the hose unit S3 and the MYC 3 unit for computer work. The laboratory unit L3 was employed for analytical work, but it was located close to the core mapping facility and not at drill site DS7.

4.2 Colloid filtering equipment

The colloid filtering equipment is adapted to the sample containers (PVB) from the PVP water sampling unit and consists of holders for two PVB-containers, a separated tube and valve system for water and gas, a filter holder package for five filters, and a collecting container. The pore sizes of the five connected filters are 0.4, 0.4, 0.2, 0.05 and 0.05 μm . The equipment is described in SKB MD 431.045 (Mätssystembeskrivning för kolloidfiltreringssystem, SKB internal controlling document to be published). Figure 4-2 shows the equipment setup.

The major equipment features are:

- Filtering is performed in a closed system under an argon atmosphere, thus avoiding the risk of iron precipitation due to contact between the groundwater sample and air.
- Filtering is performed at a pressure similar to that of the groundwater in the borehole section. The system is adjusted to create a pressure difference between the inlet of the filter package and the outlet side. The pressure difference drives the sample water through the filters.
- The design of the sample containers, and the mounting with the outlet at the top, prevents migration of larger particles which may clog the filters. Furthermore, the first two filters (pore sizes 0.4 μm) are mounted parallel to each other, also in order to prevent clogging.

Disadvantages/drawbacks, which may cause modifications to the equipment later on, are:

- The sample volume is limited to a maximum of 2×190 mL.
- The PVB sample containers are made of stainless steel which may contaminate the samples. An improvement could be to use Teflon coating on the insides of the cylindrical containers.

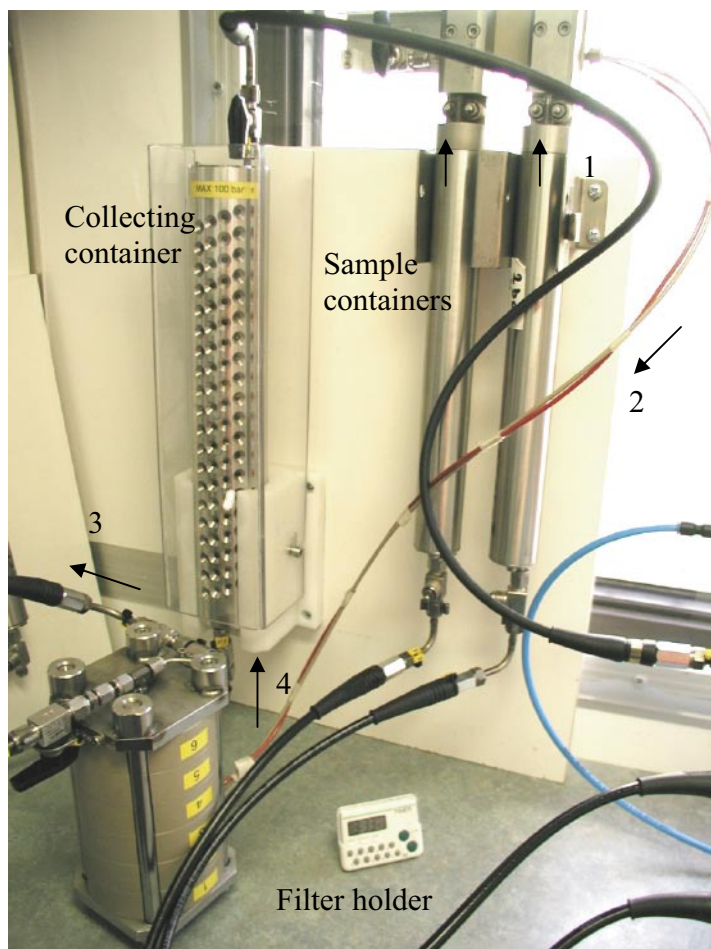


Figure 4-2. The colloid filtering equipment including the sample containers, the filter holder package and the collecting container. The black arrows, 1 to 4, show the flow direction of the sample water through the system.

4.3 Equipment for enrichment of humic and fulvic acids

Enrichment of humic and fulvic acids is conducted in order to collect enough material to determine $\delta^{13}\text{C}$ and pmC (percent modern carbon) on organic constituents in the groundwater. The equipment for enrichment includes a porous column filled with an anion exchanger (DEAE-cellulose) and a textile filter with a well-defined pore size. The textile filter is placed inside the column in order to prevent the ion exchange resin from diffusing through the column. The equipment and performance is described in SKB MD 431.044 (Mätsystembeskrivning för uppkoncentrering av humus- och fulvosyror, SKB internal controlling document). Figure 4-3 shows the equipment setup. Since the ion exchange resin in the column creates a counter-pressure, which disturbs the water flow through the surface Chemmac, a pump is used for pumping a portion of the outlet water through the column (approximately 1.8 L/hour).

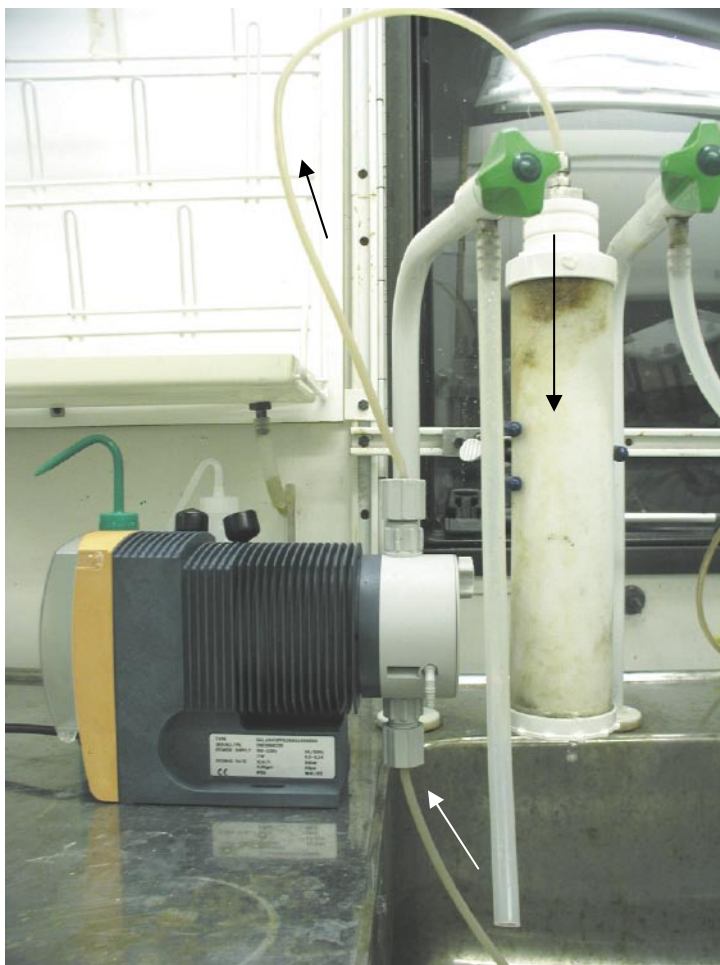


Figure 4-3. The ion exchange column. The arrows show the water flow direction.

4.4 Equipment for fractionation of humic and fulvic acids

The equipment consists of membrane filters with a defined cut-off (pore size), a membrane pump, flexible tubing and vessels. Generally, water from each section is filtered through two filters with different pore sizes (1,000 D and 5,000 D, D = Dalton, 1D = 1 g/mol). The equipment and performance are described in SKB MD 431.043 (Mätssystembeskrivning för fraktionering av humus- och fulvosyror, SKB internal controlling document). Figure 4-4 describes schematically a membrane filter and Figure 4-5 shows the complete equipment setup.

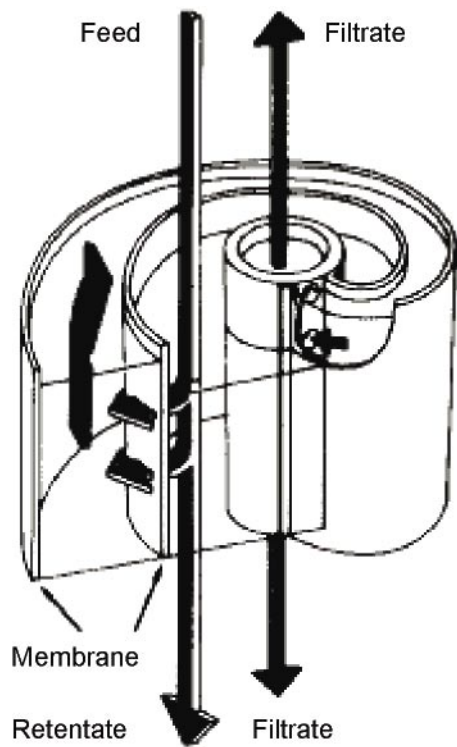


Figure 4-4. Outline of membrane filter with water flow directions.

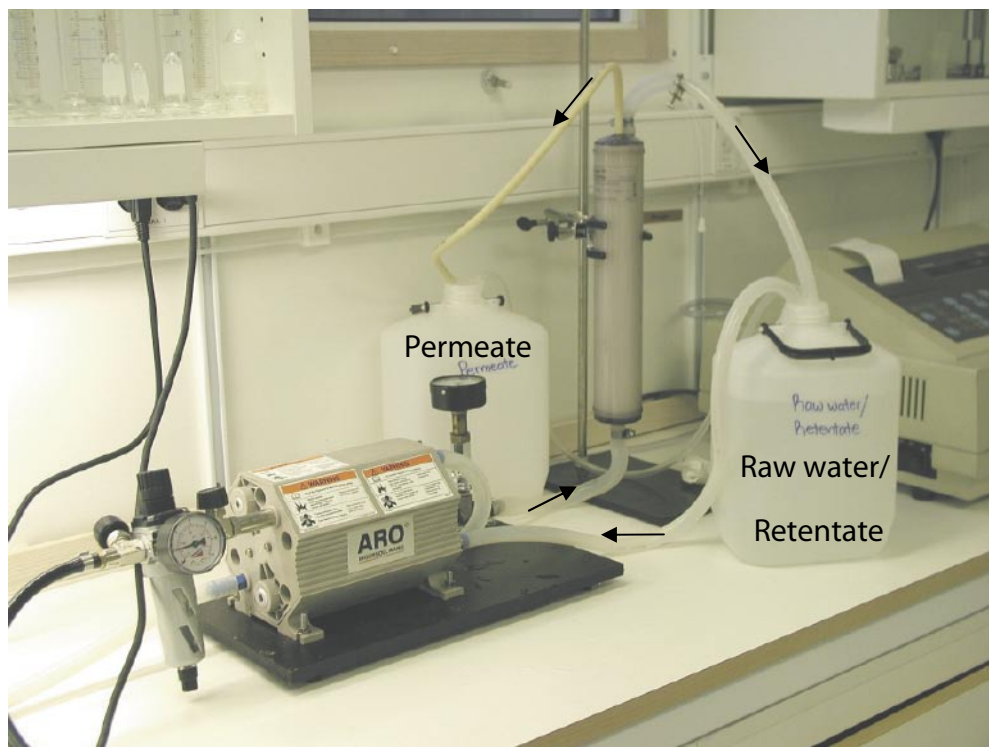


Figure 4-5. Equipment for fractionation of humic and fulvic acids.

5 Performance

5.1 General

Chemical characterisation of the section in borehole KFM07A was conducted according to activity plan AP PF 400-05-012 following the method described in SKB MD 430.017 (Metodbeskrivning för fullständig kemikaraktisering med mobilt fältlaboratorium, SKB internal controlling document). The section at 848.0–1,001.6 m was investigated from 2005-03-16 to 2005-04-26 with a total pumped volume of 10.5 m³.

5.2 Overview of field work procedure

A short chronological summary of the different steps that constitute chemical characterisation of groundwater in a borehole section is given below.

The preparations conducted before the downhole equipment is lowered in the borehole include:

- Cleaning of the inside of the umbilical hose (the sample water channel) with de-ionised, de-oxygenated water. Finally, the sample water channel is filled with de-ionised and de-oxygenated water prior to lowering.
- Cleaning and preparation of the four sample containers (PVB) belonging to the in situ water sampling unit (PVP). The containers are cleaned using 70% denatured ethanol. One of the containers is used for microbe sampling and sterile conditions are desirable. The containers are purged with nitrogen gas and a small nitrogen gas pressure is maintained in the containers. The magnitude of the pressure depends on the depth of the section to be sampled.
- Calibration of the pH and redox electrodes in the borehole Chemmac.

The different downhole units are assembled during lowering the in-the-hole equipment down the borehole, and the following steps are taken:

- The outside of the umbilical hose is cleaned with 70% denatured ethanol (SKB MD 600.004).
- Calibration of the umbilical hose length is conducted at least once for each borehole. For this purpose, a length mark detector unit (calliper) is mounted together with the ordinary in-the-hole equipment. The length mark detector indicates length calibration marks milled into the borehole wall at almost every 50 m along the borehole /3/. At each indication, a reading is made of the corresponding length mark on the umbilical hose. The correct distance to each length mark is obtained from the SICADA database.

When the pump is started and the packers are inflated at the desired positions in the borehole, a pumping and measurement period begins. Typical measures taken and activities carried out during this period are:

- Calibration of the pH and redox electrodes as well as the electrical conductivity and oxygen sensors in the surface Chemmac is conducted when the pumped water from the borehole section has reached the surface.

- Careful attention is paid to ensure that the packed-off section is well isolated from the rest of the borehole. A significant drawdown in the section during pumping is one indication that the section is properly sealed off. Leakage would cause pumping of water from the borehole column above and/or below the packers and not only from the fracture zone of interest. However, the drawdown in the borehole section must not be too large, because the greater the drawdown, the larger the bedrock volume affected by the pumping and the risk of mixing with water from other shallower and/or deeper fracture systems increases. The pumping flow rate is adjusted depending on the flow yield from the fracture or fracture zone (to between 50 and 200 mL) and maintained more or less constant during the pumping and measurement period.
- Water samples are collected regularly once or twice a week during the pumping period. Changes in water composition are monitored by conductivity measurements and by immediate analyses (chloride, pH, ferrous and total iron, alkalinity and ammonium) at the site.
- Enrichment of humic and fulvic acids is conducted for as long time as possible in each section. The time needed depends on the carbon concentration in the water and the flow rate through the ion-exchanger. Generally, a period of at least two weeks is needed to collect the amount of carbon required to determine $\delta^{13}\text{C}$ and pmC.
- Fractionation of humic and fulvic acids, as well as inorganic species to determine the size distribution, is performed at the end of the pumping period.
- A decision when to terminate the sampling work in the section is made during a suitably stable stage of the pumping and measurement period. The investigation might be prolonged if the concentration of flushing water exceeds 1% or if the redox potential measurements have not reached stable values. A final SKB Class 5 sample including all options is collected the day before termination.

Completion of the investigation in the section and lifting of the downhole equipment entails:

- Collection of in situ samples prior to lifting the equipment. The valves to the PVB sampling containers in the borehole section are opened from the surface in order to rinse the system and fill the containers. After a few hours the valves are closed and the water sample portions for analyses of colloids, dissolved gases and microbes are secured.
- Following stopping of the borehole pump and deflation of the packers, the equipment is lifted and the different downhole units are dismantled.
- Calibration of the electrodes in the borehole Chemmac and surface Chemmac.

5.3 Performance in section 848.0–1,001.6 m

The investigation carried out in section 848.0–1,001.6 m was performed with the following configuration of the in-the-hole equipment starting from the top: umbilical hose, length mark detector, borehole Chemmac, upper packer, borehole pump and in situ water sampler (PVP), see Appendix 4. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping flow rate was about 210 mL/min and the drawdown approximately 10 m. A diagram showing the pressures within and above the borehole section and the flow rate during the pumping/measurement period is given in Appendix 5. The events during the investigation are listed in Table 5-1.

Table 5-1. Events during the pumping/measurement period in section 848.0–1,001.6 m.

Date	Events Improvement/deviation	SKB sample no
050315	Calibration of borehole Chemmac. Calibration of surface Chemmac (pH and redox).	
050316	Lowering of downhole equipment (848.00–1,001.55 m). Start of Chemmac measurements.	
050317	Calibration of surface Chemmac (conductivity).	
050321	Humic and fulvic acids; enrichment start.	
050322	Water sampling: SKB class 4.	8842
050324	Water sampling: SKB class 5.	8843
050329	No flow from borehole section due to broken spring in borehole pump. Lifting.	
050330	Lowering of downhole equipment (848.00–1,001.55 m).	
050401	Water sampling: SKB class 4.	8844
050406	Water sampling: SKB class 4.	8865
050407	Water sampling: SKB class 5.	8866
050411	Water sampling: SKB class 4. Humic and fulvic acids; fractionation 5 kD.	8875 8879
050412	Humic and fulvic acids; fractionation 1 kD.	8879
050414	Water sampling: SKB class 5.	8876
050419	Water sampling: SKB class 4.	8877
050421	Water sampling: SKB class 5.	8878
050425	Water sampling: SKB class 5, all options. Humic and fulvic acids; enrichment stop. PVP-sampler: opening of valve at 10:18.	8879
050426	PVP-sampler: closure of valve at 05:41. Sampling of microbes and dissolved gases. Sampling of colloids. End of Chemmac measurements. Lifting. Calibration of borehole Chemmac. Calibration of surface Chemmac. Colloid filtration.	8879 8879
050428	Enrichment of humic and fulvic acids; eluation.	8879

5.4 Water sampling, sample treatment and analyses

The pumped water from the borehole section is conveyed from the hose unit into a container furnished with a sink and a tank for collecting the outlet water. Filtration of sample portions is performed on-line by connecting the filter holders directly to the water outlet. A water sample is defined as groundwater collected during one day and consists of several sample portions, labelled with the same sample number.

An overview of sample treatment and analysis methods is given in Appendix 7. The routines are applicable independently of sampling method or type of sampling object.

5.5 Collection of in situ water samples

The in situ water sampling in the borehole section was conducted successfully. The PVB-containers were all controlled before use; this procedure includes disassembling of the container, thorough cleaning, reassembling and measurement of piston friction.

The purpose of each sample portion is given in Table 5-2.

The PVB-containers were packed together with ice packs in insulated bags and sent by express delivery service immediately after sampling. The microbe sample arrived at the laboratory in Gothenburg before three o'clock the same day and the gas sample arrived at the laboratory in Finland the following morning. The two PVB-containers for colloid filtration were sent to the site investigation facilities in Oskarshamn where the filtration was conducted the same evening.

Table 5-2. Collection and purpose of in situ water sample portions.

Sample portion no	Section 848.0–1,001.6 m 2005-04-26
1	Dissolved gas
2	Microbes
3	Colloid filtration
4	Colloid filtration

5.6 Colloid filtration

The method for sampling colloids in groundwater entails filtering the groundwater through a series of connected filters in a closed system under an argon atmosphere. The pressure in the system is maintained at the same level as the pressure in the sampled borehole section. The intention is that colloids should be collected on the different filters (descending pore sizes) according to their sizes. Data on performance of the filtration run are given in Table 5-3. A leakage test of the system at 10 bars was also conducted prior to the sampling in order to eliminate the risk of leakage.

Each filtration results in five filter samples (two 0.4 µm, one 0.2 µm and two 0.05 µm filter pore sizes) and two water samples (water in and water out). All samples were sent for ICP analyses (major constituents and common trace metals including uranium).

Table 5-3. Colloid filtration, data on performance.

Section/date	Entering pressure (bar)	Max differential pressure over filter package (bar)	Temp (°C)	Filtering time (min)	Filtered volume (ml)	Comments
848.0–1,001.6 /20050426	~ 70.5	3.5	~ 18	27	336.5	Leakage test prior to filtration. No leakage was noticed. No broken filters

5.7 Enrichment of humic and fulvic acids

Enrichment of humic and fulvic acids was conducted in order to collect enough material to determine $\delta^{13}\text{C}$ and pmC in organic constituents in the groundwater. The method is described in SKB MD 431.044 (Mätssystembeskrivning för uppkoncentrering av humus- och fulvosyror, SKB internal controlling document). The enrichment method entails collection of organic acids on an ion exchanger, elution of the resin and evaporation of the resulting solution. The dry residue is used for isotope determination; a minimum amount of 10 mg organic carbon is needed. In addition to organic material, the residue also contains sodium hydroxide from the elution. The sample is acidified in order to prevent the formation of carbon dioxide.

Estimations of total duration time and water volume through the ion exchanger are given in Table 5-4.

Table 5-4. Enrichment time and water volume through the ion exchanger.

Borehole section (m)	Duration of enrichment (days)	Volume through ion exchanger (L)
848.0–1,001.6	28	1,036

5.8 Fractionation of humic and fulvic acids

Humic and fulvic acids were fractionated with respect to molecular weight using the ultrafiltration technique. The method is described in SKB MD 431.043 (Mätssystembeskrivning för fraktionering av humus- och fulvosyror).

Sampled water from the investigated section was first filtered through a 0.45 μm filter and then filtered through membrane filters with cut-off sizes of 1,000 D and 5,000 D, respectively. The initial water volume, prior to filtration, was approximately 5 litres. The final retentate and permeate volumes following the filtration runs were approximately 1 and 4 litres, respectively, which gave an enrichment factor of five in the retentate.

Water samples were collected from the retentate and the permeate as well as from the untreated groundwater. Each sample was analysed for dissolved organic carbon (DOC), major constituents, common trace metals and uranium. The analyses of metal ions should indicate if metals such as Al, Si, Mn, Fe and U exist as colloidal species.

6 Nonconformities

The hydrochemical characterisation in KFM07A has been conducted according to the SKB internal controlling documents AP PF 400-04-012 and SKB MD 430.017 with the following deviations and remarks:

- The investigated borehole section had to be extended compared to initial programme due to blocking by rock out-falls at approximately 850 m borehole length.
- Some equipment malfunctions have occurred during the pumping/measurement period. These are listed in Table 5-1.
- The representativity of the sampled water is uncertain /12/. Due to heavy pumping during and after the drilling, the borehole was filled to the groundwater table with very saline water which might have originated from even greater depths than 840 m (corresponding to fracture zone at 970 m borehole length).
- According to the consulted laboratory the sample resulting from the enrichment of humic and fulvic acids was not analysed ($\delta^{13}\text{C}$ and pmC) because the quality was too poor (high salt – and low organic content).
- Colloid filtration was performed at the Oskarshamn investigation site. The only available filtration system was located there when sampling was terminated in the KFM07A borehole section.

7 Data handling and interpretation

7.1 Chemmac measurement data

Processing of the Chemmac data is described in SKB MD 434.007-02 (Mätssystembeskrivning för Chemmac mätsystem, SKB internal controlling document, in progress).

7.1.1 Data file types and calculation software

The on-line measurements in a borehole section produce the following types of raw data files:

- Calibration files from calibration measurements (*.CRB) and corresponding comment files (*.CI). The files are used for calculation of calibration constants (pH and Eh) and the calibration factor (electrical conductivity). For surface Chemmac ten *.CRB and ten *.CI files are produced, and for borehole Chemmac six *.CRB and six *.CI files.
- Raw data file containing the logged measurements from the borehole section and the surface (*K.MRB) as well as a corresponding comment file (*.MI). The logged voltage values need to be converted to pH and Eh values (also in mV) using the calibration constants obtained from calibration.
- Measurement file including equipment and environment parameters (*O.MRB), such as power consumption in the downhole Chemmac unit and temperature inside the hose unit.

The original raw data files listed above are stored in the SICADA file archive. Furthermore, the files are re-calculated and evaluated to obtain pH and redox potential values and to correct the electrical conductivity values using the specially designed calculation software (Hilda). The resulting files containing calculated and evaluated values as well as comments on the performance are:

- A file **constants.mio* containing all the calculated calibration constants (one constant for each electrode in each buffer solution). The file is stored in the SICADA file archive and is useful in order to follow the development of single electrodes.
- A file **measurements.mio* containing the calculated and evaluated measurement values (pH, redox potential, electrical conductivity and water temperature). The data from the file are exported to the data tables “redox” and “ph_cond” in SICADA. As the file also contains some measured parameters that are not included in the tables mentioned above (e.g. pressure registrations) the complete file is also stored in the SICADA file archive.
- A file **comments.mio* containing comments on the fieldwork and the calculation/evaluation. The comments in the file are imported as activity comments in SICADA.

7.1.2 Calculations and evaluation of redox potential and pH

The redox potential is measured by three electrodes at the surface and three downhole in the borehole section. In addition, pH is measured by two electrodes at the surface and two downhole in the borehole section. The registrations by the redox and the pH electrodes are logged each hour during a measurement period of approximately three weeks and a calibration is performed before and after the measurement period. The treatment of the raw data includes the following steps:

- Calculation and choice of calibration constants.
- Calculation of one pH and one redox potential sequence for each electrode (i.e. three or six redox electrodes and two or four pH electrodes).
- Determination of representative pH and redox potential values as well as estimated measurement uncertainties for the investigated borehole section.

One calibration constant is selected for each electrode using one of the following alternatives:

- Case 1: Calculation of the average calibration constant value and the standard deviation. The initial and the final calibration measurements results in four constants for each redox electrode (in pH 4 and pH 7 buffer solutions) and six constants for each pH electrode (in pH 4, 7 and 10 buffer solutions).
- Case 2: The calibration constant obtained from the initial calibration measurement at pH 7 is selected since it is closest to the pH of the borehole water. This alternative is chosen if the calibration constants obtained in the different buffers show a large variation in value (generally a difference larger than 20 mV between the highest and the lowest value). The standard deviation is calculated in the same way as in Case 1.
- Case 3: If the final calibration constants turn out to be very different (more than 20 mV) from the initial constants, a linear drift correction is needed. The reason is most often a drift in the reference electrode. The values and standard deviations are calculated for the initial and the final calibration constants separately and a linear correction is made between the selected initial and the selected final constant. The higher of the two standard deviation values is used in the estimation of the total measurement uncertainty.

The values in the measurement raw data file are converted to pH and Eh measurement sequences for each pH and redox electrode using the calibration constant selected as stated above.

The next step is to choose a logging occasion in a stable part of the measurement period and select a representative result for each electrode. The average values are calculated for each electrode group in order to obtain one representative value of redox potential, pH (borehole Chemmac) and pH (surface Chemmac), respectively. Obviously erroneous electrodes are omitted. The corresponding total measurement uncertainties are estimated using the standard deviations of the calibration constants and the standard deviations of the Eh and the pH values obtained by the different sets of electrodes. It is useful to evaluate pH at the surface and pH in the borehole section separately, since pH in the pumped water might differ from the pH measured in the borehole section. This is due to changing gas pressure conditions with depth and its effects on the carbonate system.

Factors considered when evaluating the measurement uncertainties in pH and redox potential (Eh) values are:

- Difference in calibration constants for each electrode and calibration/buffer solution.
- Drift in calibration constants between the initial and the final calibration.
- Stability in voltage value during the final part of the on-line measurement. A successful measurement shows no tendency of a slope.
- Agreement between the different pH and redox electrodes on the surface and in the downhole borehole Chemmac.
- Number of electrodes showing reasonable agreement. Obviously erroneous electrodes are excluded from the calculation.

7.2 Water analysis data

The following routines for quality control and data management are generally applied for hydrogeochemical analysis data, independently of sampling method or sampling object.

Several components are determined by more than one method and/or laboratory. Moreover, duplicate analyses by an independent laboratory are performed as a standard procedure on each fifth or tenth collected sample. All analytical results are stored in the SICADA database. The applied hierarchy path “Hydrochemistry/Hydrochemical investigation/Analyses/Water in the database” contains two types of tables, raw data tables and primary data tables (final data tables).

Data on basic water analyses are inserted into the raw data tables for further evaluation. The evaluation results in a final reduced data set for each sample. These data sets are compiled in a primary data table named “water composition”. The evaluation is based on:

- Comparison of the results from different laboratories and/or methods. The analyses are repeated if a large disparity is noted (generally more than 10%).
- Calculation of charge balance errors according to the equation below. Relative errors within $\pm 5\%$ are considered acceptable (in surface waters $\pm 10\%$).

$$\text{Relative error (\%)} = 100 \times \frac{\sum \text{cations}(\text{equivalents}) - \sum \text{anions}(\text{equivalents})}{\sum \text{cations}(\text{equivalents}) + \sum \text{anions}(\text{equivalents})}$$

- General expert judgement of plausibility based on earlier results and experience.

All results from special analyses of trace metals and isotopes are inserted directly into primary data tables. In those cases where the analyses are repeated or performed by more than one laboratory, a “best choice” notation will indicate those results which are considered most reliable.

An overview of the data management is given in Figure 7-1.

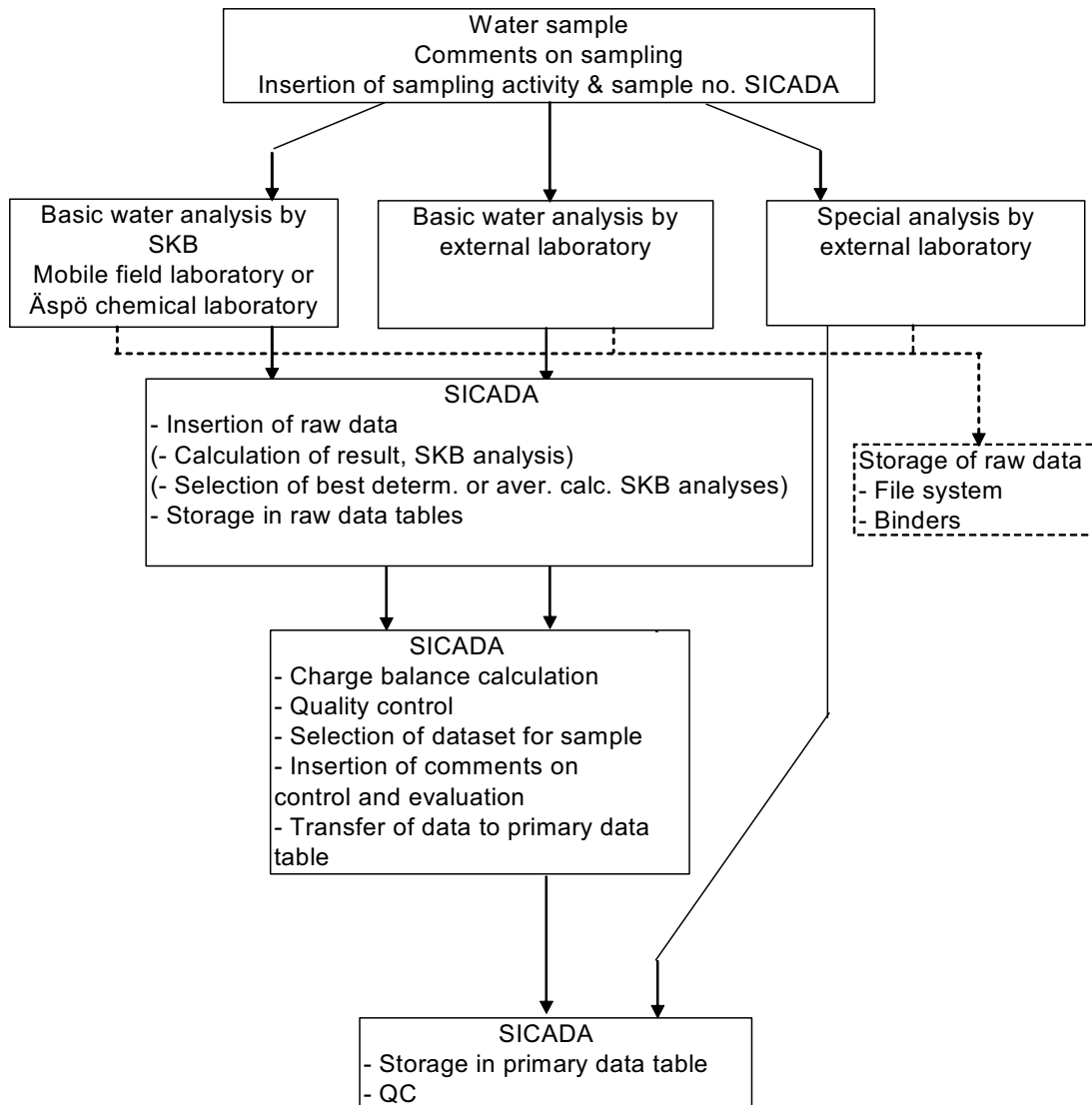


Figure 7-1. Overview of data management for hydrogeochemical data.

7.3 Data from special sampling methods

Special sampling methods include collection of in situ samples (colloid filtration, and dissolved gases), enrichment and fractionation of humic and fulvic acids.

Separate sampling activities, methods and sample numbers are defined for data on dissolved gases, colloids, fractions of humic and fulvic acids and $\delta^{13}\text{C}$ and pmC determined on organic constituents. All analytical data are subjected to quality control and stored in the SICADA database.

7.3.1 Colloid filtration

The concentration of the colloid portion caught on each filter is calculated with the assumption that the water volume coming out in the collecting container is equal to the volume going into the system. This is not quite true as up to ten millilitres will be left in cavities in the filter holder package, in the tubing and in valves. A small volume of about 0.01 to 0.06 mL is left in each filter after the filtration and its content of the different elements is included in the analysis. The measurement uncertainty of each concentration is calculated according to the equation below.

$$U = \sqrt{\left(\frac{1}{V^2} \cdot (\Delta m)^2 + \frac{m^2}{V^4} (\Delta V)^2 \right)}$$

where

- U = measurement uncertainty (µg/L)
- V = water volume through the system (L)
- ΔV = estimated volume error, 0.010 L
- m = amount on filter (µg)
- Δm = measurement uncertainty of the filter analysis, 20% (µg)

The results from the filter analyses are stored in SICADA.

7.3.2 Dissolved gases

Results from gas analyses are stored in a primary data table in SICADA without post processing or interpretations.

7.3.3 Enrichment of humic and fulvic acids

The pmC and δ¹³C values for enriched organic acids are stored in SICADA without post processing or interpretations.

7.3.4 Fractionation of humic and fulvic acids

The concentrations of organic and inorganic constituents in the retentate and permeate are recalculated to concentrations of each fraction of carbon and metal ions with molecular weight lower or higher than the cut-off size of the filter. This is done using mass balance equations as described in SKB MD 431.043, (Mätssystembeskrivning för fraktionering av humus- och fulvosyror. Comparison of the four concentration values from the two filters results in values for three fractions, i.e. < 1,000 D, 1,000–5,000 D and > 5,000 D.

8 Results

8.1 Chemmac measurements

The measured sequences (Eh, pH, electrical conductivity, oxygen and temperature) from the Chemmac measurements in section 848.0-1,001.6 m are presented in diagrams in Appendix 6. The six redox electrodes reached stable values that coincided quite well but the fact that the Eh-values turned out to be positive is difficult to explain. Both pH-electrodes at the ground surface agree completely but showed a regular 24 hour variation between night and day. This was traced to unacceptable temperature variations in the hose unit. The two in situ pH-electrodes differ by approx 0.2 pH units. The calibration of the PHB electrode was less reliable and therefore these data were rejected. The in- and out-calibrations of the PHIB electrode, on the other hand, showed agreement from each of the three buffers.

The measured monitoring time series data were evaluated in order to obtain one representative value of Eh, pH, electrical conductivity and dissolved oxygen for the borehole section as described in Section 7.1. Data were selected from a part of the measured time series sequences where the electrodes show stable values, marked with an arrow in the plots in Appendix 6. The evaluated results from the measurements in the investigated section are given in Table 8-1.

Table 8-1. Evaluated results from the Chemmac measurement in KFM07A.

Borehole section (m)	Electrical conductivity* (mS/m)	pH (surface Chemmac)**	pH (borehole Chemmac)**	Eh (borehole and surface Chemmac)** (mV)	Dissolved oxygen*** (mg/L)
848.0–1,001.6	3,630 ± 110	8.05 ± 0.15	8.04 ± 0.38	9.39 ± 6.56	0.00 ± 0.01

*The electrical conductivity is measured between 0–10 000 mS/m with a measurement uncertainty of 3%.

** Evaluated result and measurement uncertainty calculated as described in Section 7.1.

*** Measuring interval 0–15 mg/L, resolution 0.01 mg/L.

8.2 Water analyses

8.2.1 Basic water analyses

The basic water analyses include the major constituents Na, K, Ca, Mg, S, Sr, SO₄²⁻, Cl⁻, Si and HCO₃⁻ as well as the minor constituents Fe, Li, Mn, DOC, Br, F, I, HS⁻ and NH₄⁺. Furthermore, batch measurements of pH and electrical conductivity are included. Another important parameter is the flushing water content in each sample. The basic water analysis data and relative charge balance errors are compiled in Appendix 8, Table A8-1. Existing batch measurement values of pH and electrical conductivity are compared to the corresponding on-line Chemmac measurement values in Appendix 6.

The charge balance errors give an indication of the quality and uncertainty of the analyses of major constituents. The errors do not exceed ± 5% in any case. Furthermore, the last sample in each section was also analysed by an independent laboratory. A comparison between results from different laboratories and methods shows that the agreement is acceptable in most cases. Generally, the difference in concentrations between laboratories/methods for each analysed constituent is less than 10%.

The flushing water contents in the sample series collected from the borehole sections are presented in Figure 8-1. The content should not exceed 1% in order for a sample to be considered representative for the groundwater of the sampled fracture zone. This condition was met for samples collected in section 848.0–1,001.6 m. The flushing water contents are calculated using the nominal Uranine concentration (0.20 mg/L) in the flushing water.

The concentration levels of sodium, calcium and chloride are presented in Figure 8-2. The concentrations of all major constituents remained practically constant during the pumping and sampling period.

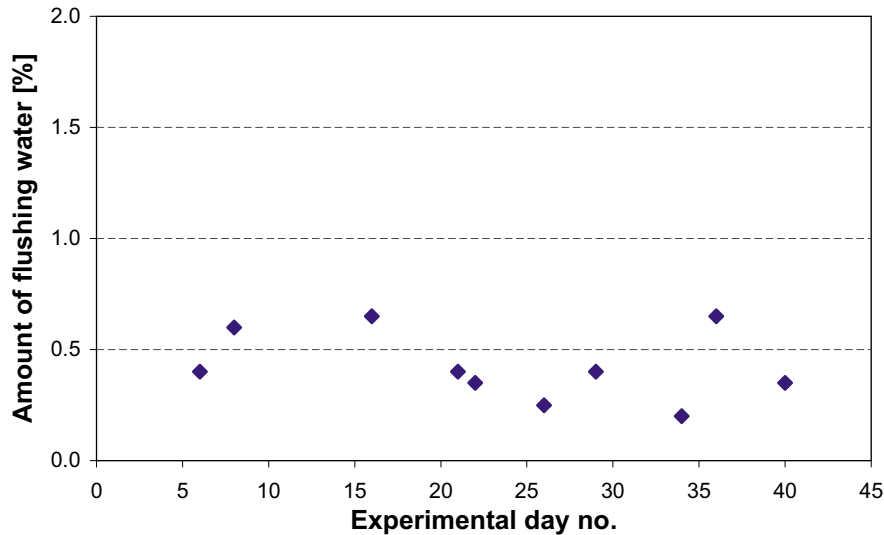


Figure 8-1. Flushing water content versus experimental day number, section 848.0–1,001.6 m.

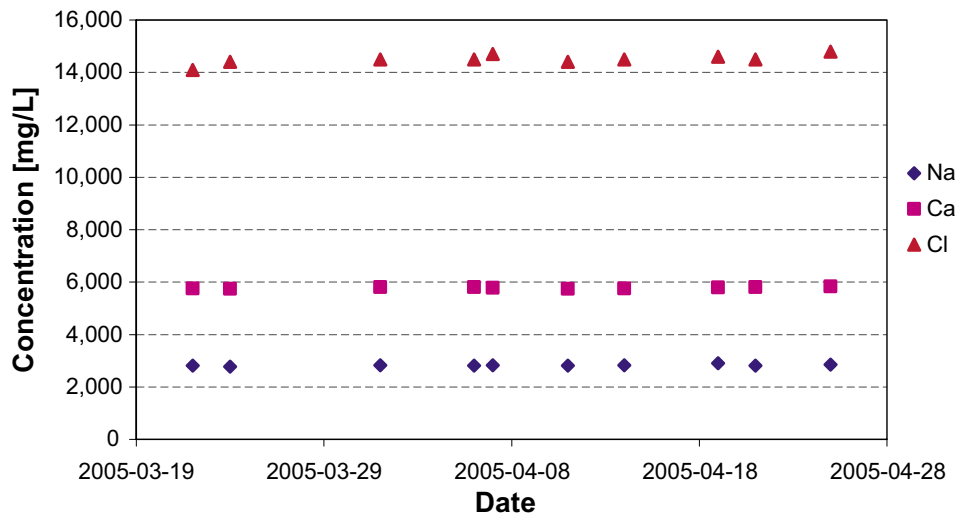


Figure 8-2. Sodium, calcium and chloride concentrations from sample series at 848.0–1,001.6 m.

The iron concentrations determined by ICP-AES (total Fe) and by spectrophotometry (Fe(+II) and Fe-tot) are compared in Figure 8-3. The total iron concentrations determined by ICP agree well with the results obtained by spectrophotometry. The iron concentrations show a slowly decreasing trend throughout the sampling period.

Sulphate analysed by ion chromatography (IC) is compared to sulphate determined as total sulphur by ICP-AES in Figure 8-4. As shown, the ICP-values are somewhat higher than the IC results. Sulphide driven off as hydrogen sulphide gas into the plasma may in these cases contribute to the ICP result. From experience, the results from the ICP measurements are, however, considered more reliable, since the variation between samples in a time series often is smaller. The sulphate concentration remained constant during the sampling period.

For rough check of data, the chloride concentrations are plotted versus the corresponding electrical conductivity values in Figure 8-5. As shown, the data from the borehole sections agree well with a regression line obtained by earlier data from the Äspö Hard Rock Laboratory.

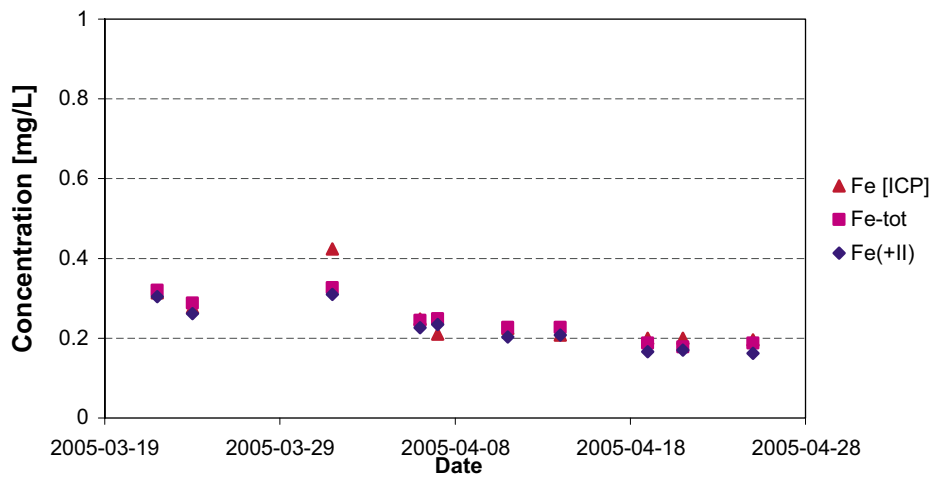


Figure 8-3. Comparison of iron concentrations obtained by ICP-AES and by spectrophotometry, borehole section 848.0–1,001.6 m.

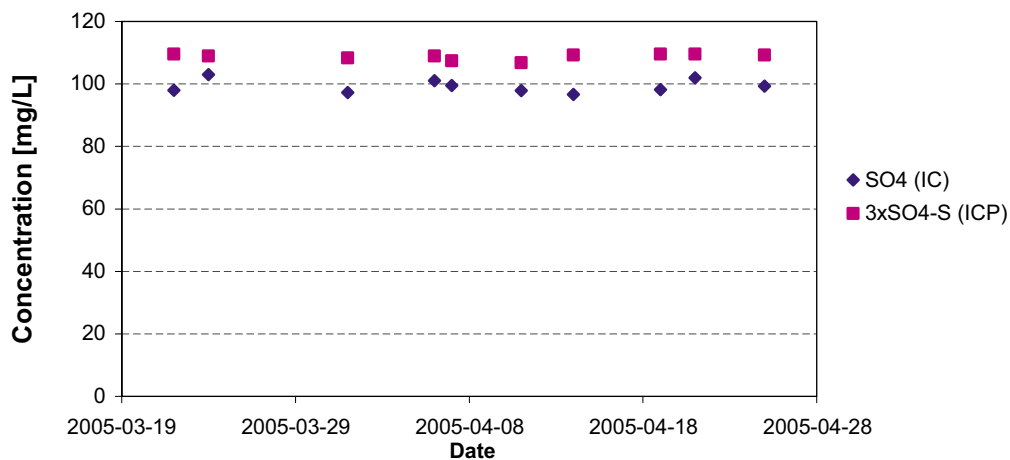


Figure 8-4. Sulphate (SO_4 by IC) to total sulphate calculated from total sulphur ($3 \times SO_4-S$ by ICP) versus date, borehole section 848.0–1,001.6 m.

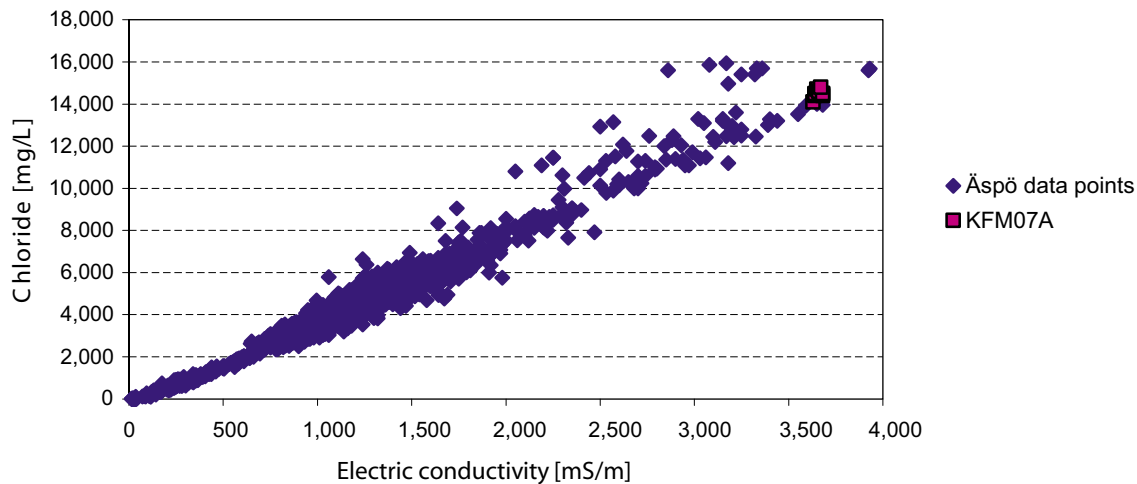


Figure 8-5. Chloride concentration versus electrical conductivity. Data from earlier investigations at the Äspö Hard Rock Laboratory are used to show the linear trend. Data from KFM07A do not deviate significantly from a thought regression line.

8.2.2 Trace elements (rare earth metals and others)

The analyses of trace and rare earth metals include U, Th, Sc, Rb, Y, Zr, In, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu. Commonly occurring metals, such as Cu, Zn, Pb and Mo are not included in the analysis programme due to contamination considerations. As can be seen from the following Tables 8-3 and 8-4, the risk of contamination is large also for aluminium. The aluminium concentration is still reported due to its importance for the modelling work. The trace element data are compiled in Appendix 8, Table A8-3.

8.2.3 Stable and radioactive isotopes

The isotope determinations include the stable isotopes δD , $\delta^{18}O$, $^{10}B/^{11}B$, $\delta^{34}S$, $\delta^{13}C$, ^{37}Cl and $^{87}Sr/^{86}Sr$ as well as the radioactive isotopes Tr (TU), ^{14}C (pmC), ^{238}U , ^{235}U , ^{234}U , ^{232}Th , ^{230}Th , ^{226}Ra and ^{222}Rn . Available isotope data at the time of reporting are compiled in Appendix 8, Table A8-2 and Table A8-4.

The carbon isotopes ($\delta^{13}C$ and pmC) were determined in inorganic carbon (hydrogen carbonate) but not in organic constituents.

8.3 Dissolved gas

The analyses of dissolved gases include argon (Ar), helium (He), nitrogen (N_2), carbon dioxide (CO_2), methane (CH_4), oxygen (O_2), carbon monoxide (CO), hydrogen (H_2), ethane (C_2H_6), ethene (C_2H_4), ethyne (C_2H_2), propane (C_3H_8) and propene (C_3H_6). The gas data are compiled in Appendix 8, Table A8-5.

Total gas content in the groundwater as well as the detected oxygen content are given in Table 8-2. The oxygen content indicates air leakage into the purging system at the consulted laboratory. The results may be corrected by removing the air effect (nitrogen, oxygen and argon) assuming that the oxygen content is zero.

The gas composition of the groundwater in borehole section 848.0–1,001.6 m is presented in Figures 8-6 and 8-7.

Table 8-2. Total content of dissolved gas.

	Section 848.0–1,001.6 m
Total gas content (mL/L)	161
Oxygen content (mL/L)	0.19

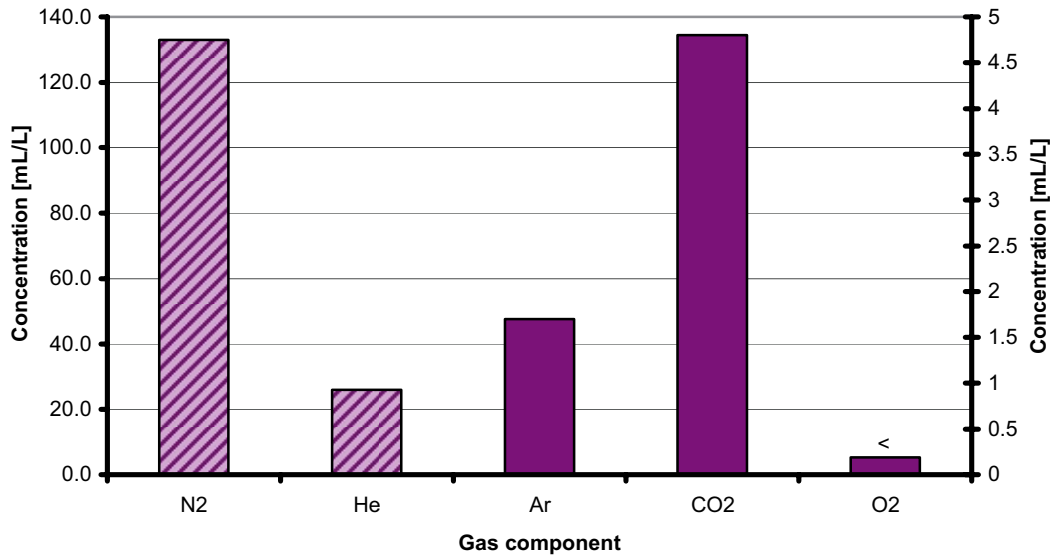


Figure 8-6. Gas components (N₂, He, Ar, CO₂, and O₂) of high concentrations in samples collected in borehole section 848.0–1,001.6 m. Striped and unstriped bars refer to the left and right axis, respectively.

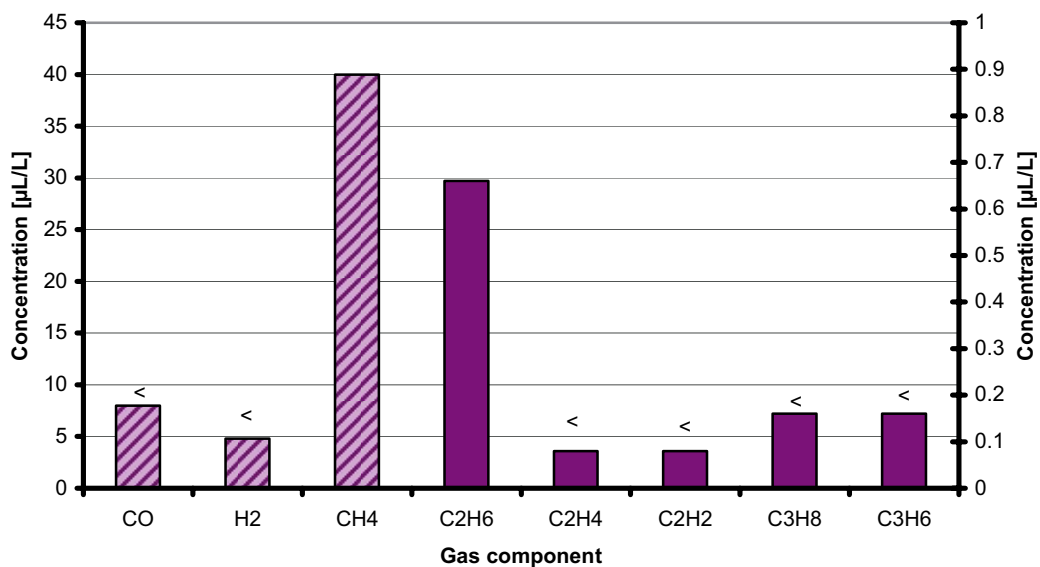


Figure 8-7. Gas components (CO, H₂, CH₄, C₂H₆, C₂H₄, C₂H₂, C₃H₈ and C₃H₆) of low concentrations in samples collected in borehole section 848.0–1,001.6 m. Striped and unstriped bars refer to the left and right axis, respectively.

8.4 Inorganic colloids

The presence of inorganic colloids was investigated by two standard methods, 1) filtration through a series of connected filters of different pore sizes, and 2) fractionation/ultra filtration using two cylindrical membrane filters with a cut-off of 1,000 D and 5,000 D, respectively. The results of the two methods are difficult to compare quantitatively but a qualitative agreement was indicated.

8.4.1 Inorganic colloids – colloid filtration

The results from the colloid filtration method conducted in sections 848.0–1,001.6 are presented in Figures 8-8 to 8-14.

The bars in the diagrams represent amounts (μg) of aluminium, iron, silicon manganese and uranium entering the filter package, incorporated on each filter and present in the collecting container. The amounts are calculated assuming that the water volume coming out from the filter package and into the collecting container is equal to the volume going into the system. This is not quite the case, as up to ten millilitres will be left in cavities in the filter holder package, in the tubing and in valves. Further, a small volume of about 0.01 to 0.06 mL is left in each filter after the filtration and the salt content of this volume is included in the analysis. The presented input amounts, in the diagrams below, represent the sample collected on-line at the surface just before opening the PVB-containers for sampling.

Analysis of blank filters showed that the contributions of aluminium, iron, silica, manganese and uranium from the filters were insignificant.

The following conclusions may be drawn from the colloid filtration results:

- Aluminium results are somewhat difficult to evaluate since the output amount plus the amounts incorporated on filters do not balance the input amount. As can be concluded from Table 8-3, the reasons are contamination and/or precipitation in the PVB-containers. The imbalance of aluminium may also be due to analytical uncertainty, since the concentrations are low.
- Calcium is present at high concentration in ground water and water volumes left to dry in the filters will provide significant contribution to the filter analyses. A remaining sample volume of 0.06 mL gives a calcium contribution of approximately 0.3 mg to the filter.
- Aluminium, iron and possibly calcium are detected in significant amounts on the filters. Addition of corresponding amounts of aluminium as K-Mg-illite and $\text{Fe}(\text{OH})_2$ (0.4 μm filter pore size excluded) results in a colloid concentration of approximately 10 $\mu\text{g}/\text{L}$. It is most probable that real background concentration is significantly lower, because precipitated iron as well as contamination by iron and aluminium contributes.

Results of colloid filtering experiment, using water sample from section 848.0-1001.6 m

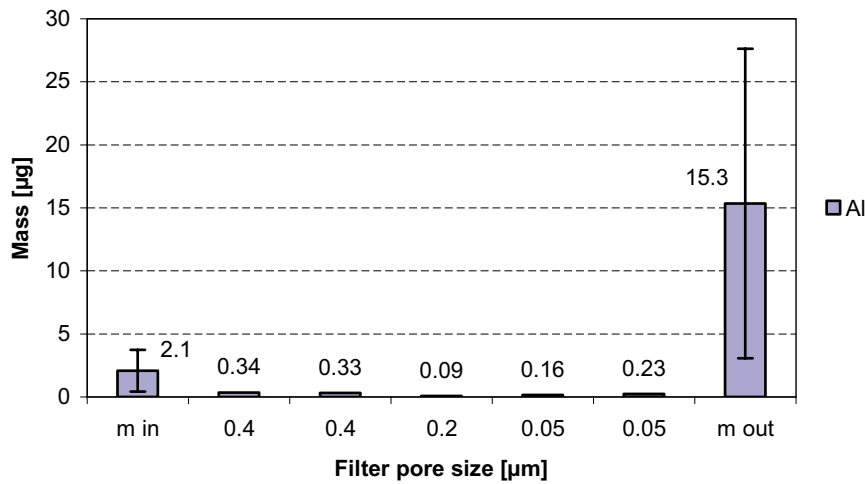


Figure 8-8. Amount of aluminium entering the filter system (m in), in the filters and in the collecting container (m out).

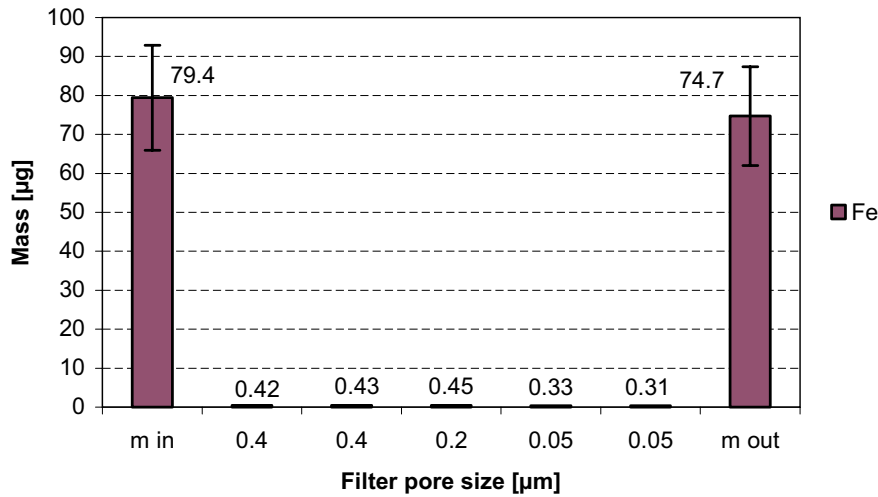


Figure 8-9. Amount of iron entering the filter system (m in), in the filters and in the collecting container (m out).

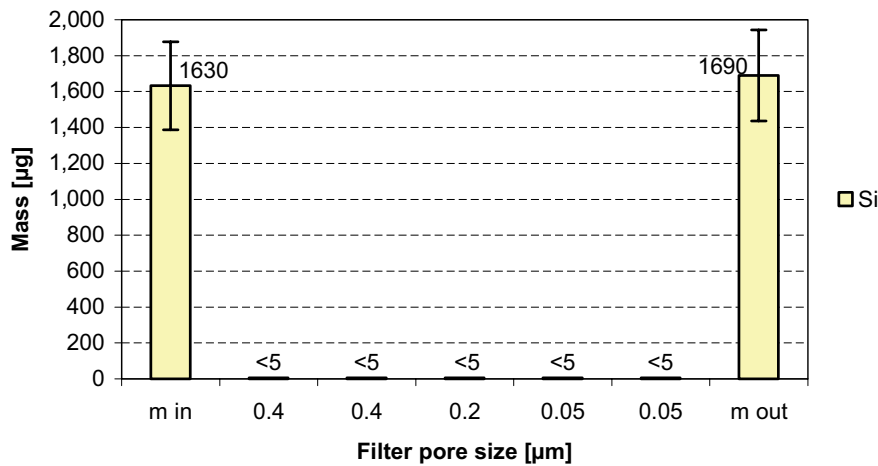


Figure 8-10. Amount of silicon entering the filter system (m in), in the filters and in the collecting container (m out).

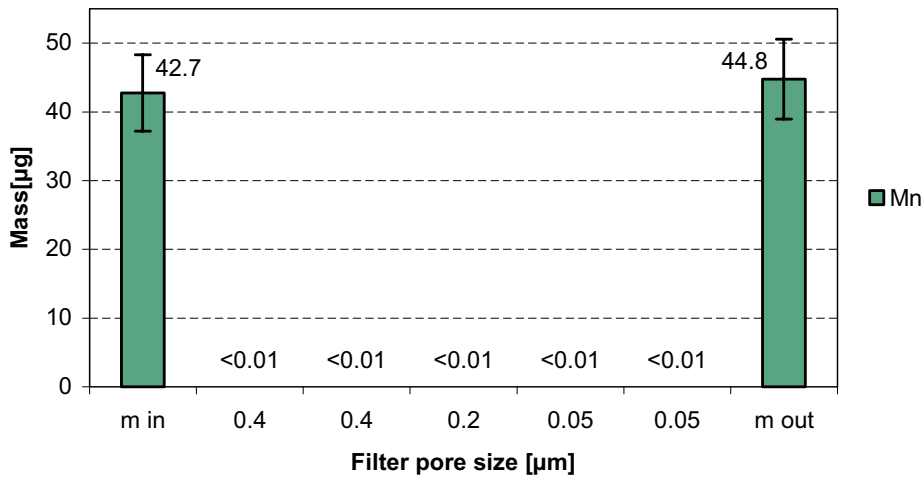


Figure 8-11. Amount of manganese entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

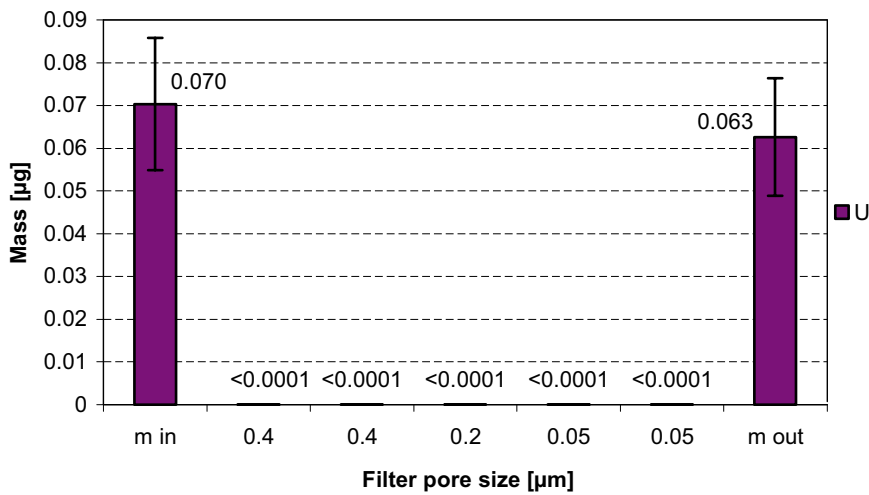


Figure 8-12. Amount of uranium entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

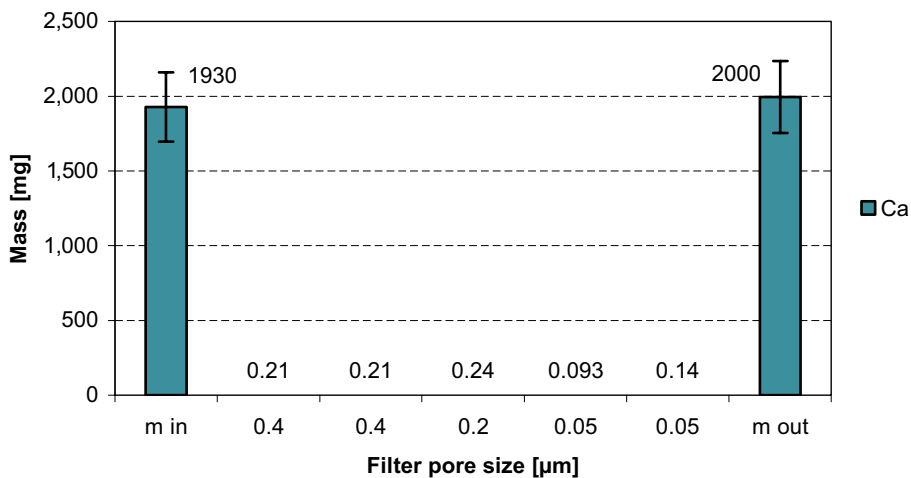


Figure 8-13. Amount of calcium entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

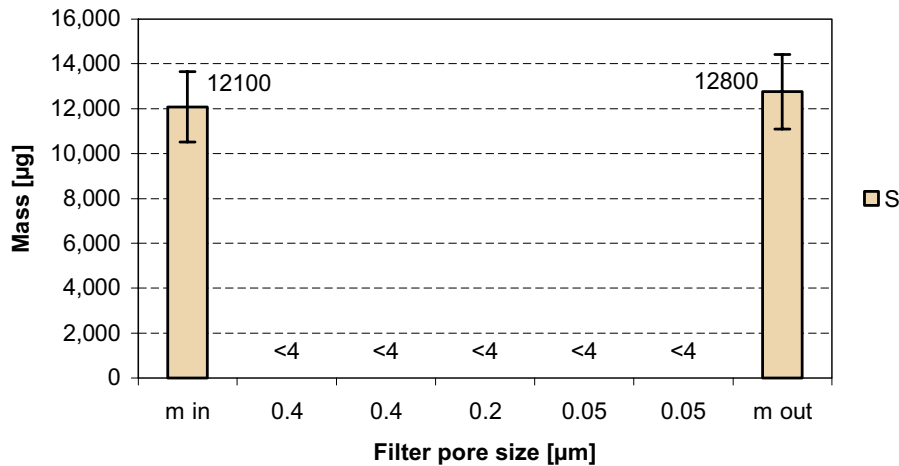


Figure 8-14. Amount of sulphur entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

Table 8-3. Element concentrations in; de-ionised water, blank water, remaining water in PVB container, collected output water from filter system and pumped water that has not passed the filter system.

Sample origin	Al µg/L	Ca mg/L	Fe mg/L	Mn µg/L	Si mg/L	S mg/L	U µg/L
Deionised water	0.829	< 0.1	0.001	< 0.03	0.0924	< 0.2	–
Blank	1.52	0.1	0.0068	0.426	0.849	0.559	0.0015
Rest volume PVB (input conc)	7,420	5,830	1.87	170	17.3	36.8	0.977
	18,600	5,950	4.48	240	35.3	36.7	1.96
Collecting container	45.6	5,930	0.222	133	5.02	37.9	0.186
Pumped water (alt. input conc)	6.19	5,730	0.236	127	4.85	35.9	0.209

Deionised water = from the tap.

Blank = deionised water used as rinsing water, leakage test.

Rest volume PVB = remaining water in the PVB container after filtering experiment.

Collecting container = water that has passed the filter system.

Pumped water = ordinary sample collected at the surface and not in situ in the borehole section.

– = no analysis.

8.4.2 Inorganic colloids – fractionation

Besides the DOC analyses, the samples from the fractionation experiment were analysed by ICP-AES and ICP-MS. The determined elements were; Ca, Fe, K, Mg, Na, S, Si, Al, Ba, Cd, Co, Cr, Cu, Hg, Li, Mn, Mo, Ni, P, Pb, Sr, V, Zn and U. Only iron, silicon, aluminium, calcium, manganese, uranium and sulphur were considered important as colloid species.

The results presented in Table 8-3 were calculated using mass balance equations (SKB MD 431.043). As shown, Si, Al, Mn, Ca, U and S exist as species (associated or non-associated with humic and fulvic acids) with a molecular weight less than 1,000 g/mol. Such species are too small to be referred to as colloids. The iron results were inconsistent, possibly due to omitted acid addition, and are therefore rejected.

The filters were carefully washed before use and samples of de-ionised water (after passing through the washed filters) were analysed as sample blanks. The concentrations of analysed elements were below the detection limits.

The results do not indicate any precipitation of calcite during the filtrations.

Table 8-4. Inorganic size fractions (1,000 D and 5,000 D filters), section 848.0–1,001.6 m.

Fraction	Fe (mg/L)	Si (mg/L)	Al (µg/L)	Mn (µg/L)	Ca (mg/L)	U (µg/L)	S (mg/L)
< 1,000 D	NR	4.5 ± 0.7	12.1 ± 8.5	134 ± 23	5,480 ± 658	0.22 ± 0.03	33.5 ± 3.4
< 5,000 D	NR	4.6 ± 0.7	2.6 ± 1.8	135 ± 23	5,530 ± 664	0.18 ± 0.03	33.6 ± 3.4
> 1,000 D but < 5,000 D	NR	–	–	–	–	–	–
> 5,000 D	NR	–	–	–	–	–	–
Adsorption 1,000 D	NR	–	–	–	–	–	–
Adsorption 5,000 D	NR	–	–	–	–	–	–

– = Not found.

NR = Not reported due to inconsistent results.

8.5 Humic and fulvic acids

The result from fractionation of organic acids in section 848.0–1,001.6 m is summarised in Table 8-4. If there is a low concentration of organic acids in the groundwater, it is present as low molecular weight fulvic acids or other low molecular weight organic acids such as citric acid and oxalic acid with a molecular weight less than 1,000 D.

Table 8-4. Summary of fractionation results.

Fraction	Section 848.0–1,001.6 m DOC (mg/L)
< 1,000 D	< 1.0
> 1,000 D but < 5,000 D	–
> 5,000 D	–

– = Not found.

The results from the 1,000 D and 5,000 D filters were consistent.

9 Summary and discussion

The chemical characterisation of the deep borehole section 848.0–1,001.6 m in KFM07A was performed without major technical problems. However, a complicating factor concerning the borehole that needs to be addressed when evaluating the borehole data is the uncertainty about the depth of origin of the sampled water. In KFM07A the heavy pumping during and after drilling has almost filled the entire borehole with saline water that may represent greater depths than 840 m (corresponding to fracture zone at 970 m borehole length) demarcated for sampling /11/. Figure 9-1 presents the chloride versus depth dependence of groundwaters from KFM07A and other current boreholes at Forsmark. The diagram suggests that the increase in chloride concentration below c. 600 m is steeper in the prioritised northwestern part of the candidate area than in the south (KFM03A).

The main conclusions from the experimental results are:

- An upper limit for the allowed flushing water content in a representative water sample is set to 1%. This requirement was fulfilled in section 848.0–1,001.6 m (0.5%).
- The water composition was stable during the pumping/sampling period. A low magnesium to chloride ratio indicates a deep saline groundwater type of non marine origin.
- It is not plausible that the positive redox potential value measured in the borehole section is representative for undisturbed groundwater at this depth. However, the result is difficult to explain as no electrode malfunction is observed. It cannot be excluded that the explanation is related to the observed up-coning effect due to heavy pumping during and after drilling.

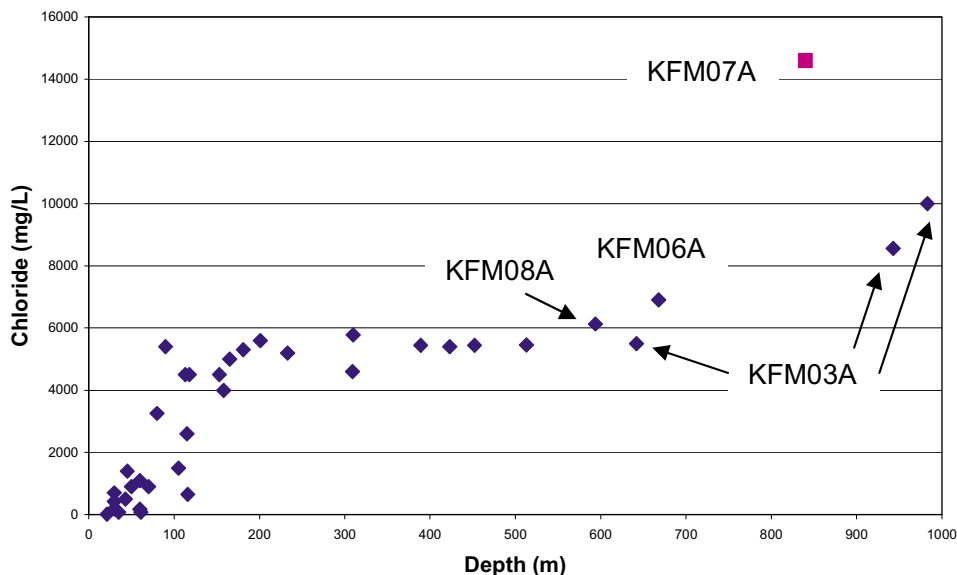


Figure 9-1. Chloride concentration in the groundwater versus depth at Forsmark. Available data at the time being are included.

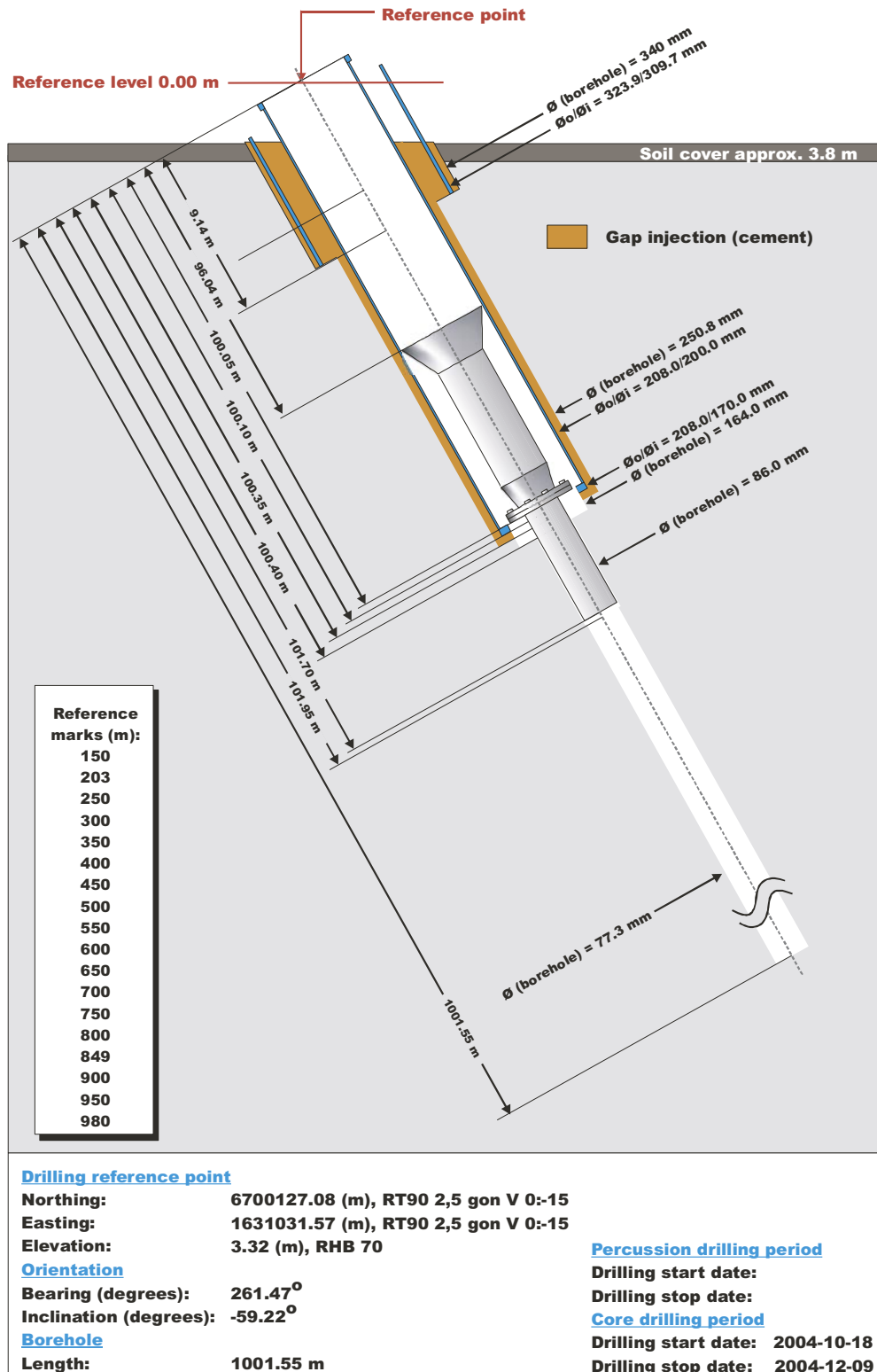
- The fractionation experiment showed that the studied elements (Al, Fe, Mn, Ca, U and S) were present as low molecular weight species. On the other hand, the colloid filtering results indicate significant amounts of aluminium and iron incorporated on the filters. Addition of corresponding amounts of aluminium as K-Mg-illite and $\text{Fe}(\text{OH})_2$ (0.4 μm filter pore size excluded) gives a colloid concentration of approximately 10 $\mu\text{g/L}$. It is most probable that the real background concentration is significantly lower, because precipitated iron as well as contamination by iron and aluminium may contribute.
- If organic constituents exist in the groundwater, they are present as low molecular weight fulvic acids or other low molecular weight organic acids such as citric acid and oxalic acid with a molecular weight less than 1,000 D.

10 References

- /1/ **SKB, 2001.** Site investigations. Investigation methods and general execution programme. SKB TR-01-29, Svensk Kärnbränslehantering AB.
- /2/ **Pedersen K, 2005.** Forsmark site investigation. Numbers and metabolic diversity of microorganisms in boreholes KFM06A and KFM07A. Results from sections 353.5–356.6 and 768–775 m in KFM06A and section 848–1,001.6 m in KFM07A. SKB P-05-177, Svensk Kärnbränslehantering AB.
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- /4/ **SKB, 2005.** Forsmark site investigation. Programme for further investigations of geosphere and biosphere. SKB R-05-14, Svensk Kärnbränslehantering AB.
- /5/ **Claesson L-Å, Nilsson G, 2005.** Forsmark site investigation. Drilling of two flushing water wells, HFM21 and HFM22, one groundwater monitoring well in solid bedrock, HFM20, and one groundwater monitoring well in soil, SFM0076. SKB P-04-245, Svensk Kärnbränslehantering AB.
- /6/ **Nilsson D, 2005.** Forsmark site investigation. Sampling and analyses of groundwater from percussion drilled boreholes. Results from the percussion drilled boreholes HFM20, HFM21 and HFM22. SKB P-05-48, Svensk Kärnbränslehantering AB.
- /7/ **Pedersen K, Kalmus A, 2003.** Forsmark site investigation. Control of microorganism content in flushing water used for drilling of KFM06A. SKB P-04-285, Svensk Kärnbränslehantering AB.
- /8/ **Gustafsson J, Gustafsson C, 2005.** Forsmark site investigation. RAMAC and BIPS logging in borehole KFM07A. SKB P-05-52, Svensk Kärnbränslehantering AB.
- /9/ **Rouhiainen P, Sokolnicki M, 2005.** Forsmark site investigation. Differential flow logging in borehole KFM07A. SKB P-05-63, Svensk Kärnbränslehantering AB.
- /10/ **Nielsen U T, Ringgard J, Fris Dahl J, 2005.** Forsmark site investigation. Geophysical borehole logging in the boreholes KFM07A, KFM08A and KFM08B. SKB P-05-159, Svensk Kärnbränslehantering AB.
- /11/ **Gokall-Norman K, Svensson T, Ludvigsson J-E, 2005.** Forsmark site investigation. Single-hole injection tests in borehole KFM07A. SKB P-05-133, Svensk Kärnbränslehantering AB.

Design of cored borehole KFM07A

Technical data Borehole KFM07A



Selected results from differential flow logging

Forsmark, borehole KFM07A
Transmissivity and head of 5 m sections

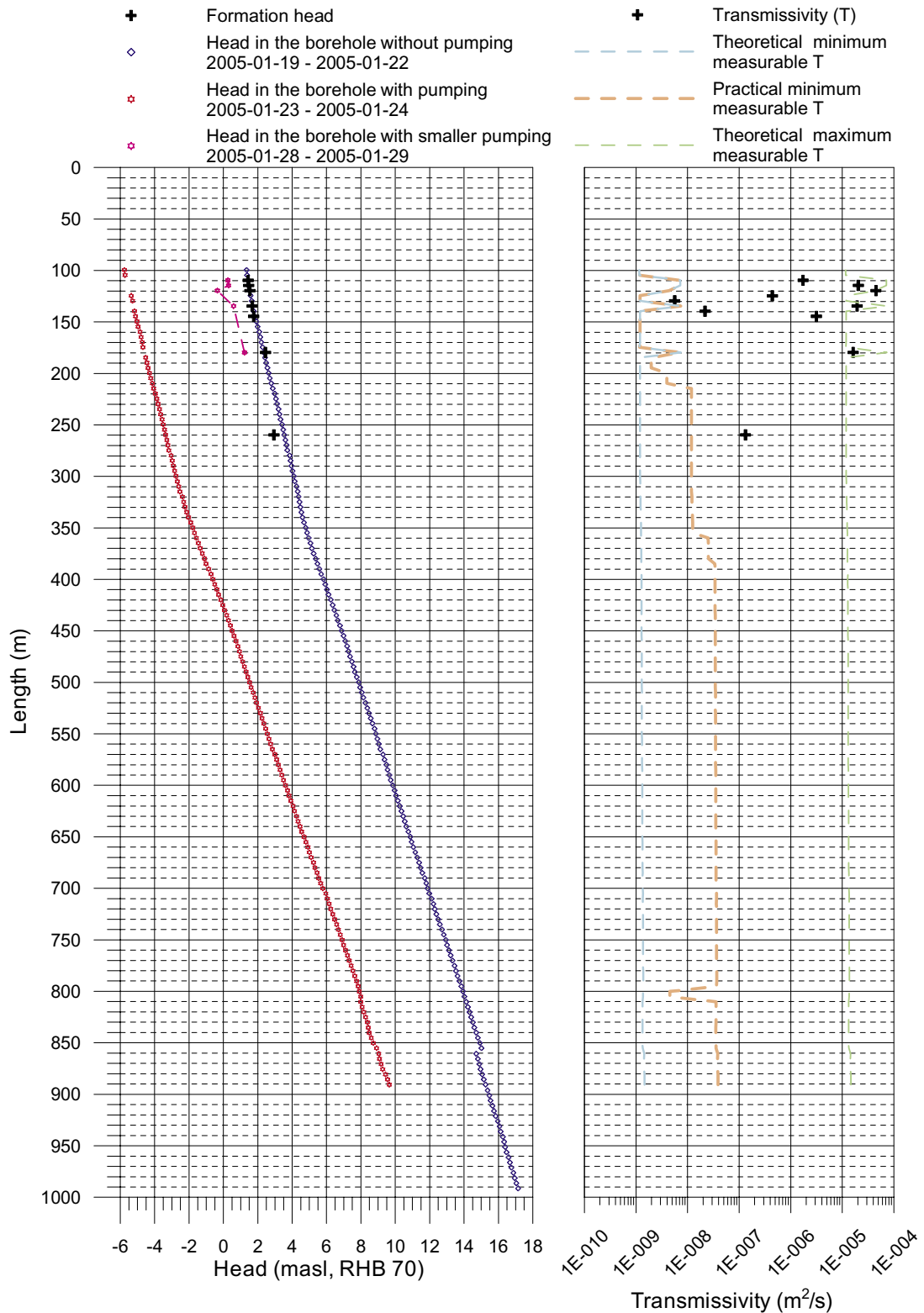


Figure A2-1. Borehole KFM07A: head and transmissivity of 5 m sections /9/.

Forsmark, borehole KFM07A
 Measured flow rates, caliper and single point resistance

- △ Without pumping (L=5 m, dL=5 m), (Flow direction = into the hole)
- ▽ Without pumping (L=5 m, dL=5 m), (Flow direction = into the bedrock)
- △ With pumping (L=5 m, dL=5 m), (Flow direction = into the hole)
- Without pumping (L=5 m, dL=0.5 m) REP1, 2005-01-19 - 2005-01-20
- Without pumping (L=5 m, dL=0.5 m) REP2, 2005-01-21 - 2005-01-22
- With pumping (L=5 m, dL=0.5 m), 2005-01-23 - 2005-01-24
- With pumping (L=1 m, dL=0.1 m), 2005-01-25 - 2005-01-27
- With smaller pumping (L=1 m, dL=0.1 m), 2005-01-28 - 2005-01-29
- — — Lower limit of flow rate

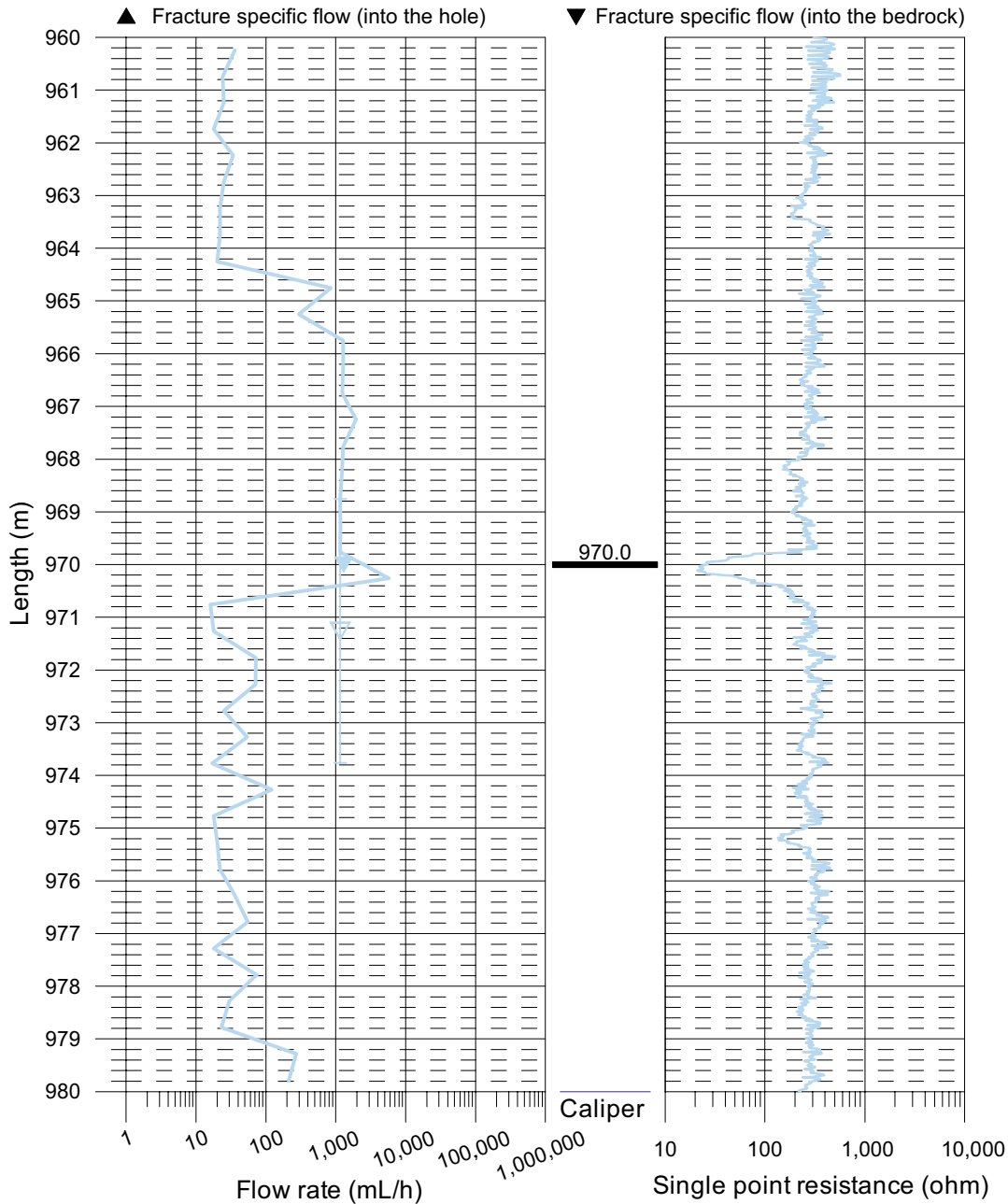


Figure A2-2. Borehole KFM07A: differential flow measurements from 960 to 980 m including the water bearing fracture zone at approx 970 m [9]. This part of the borehole was only logged without pumping due to blocking by rock out-falls that occurred later on.

Selected BIPS logging image at 970 m

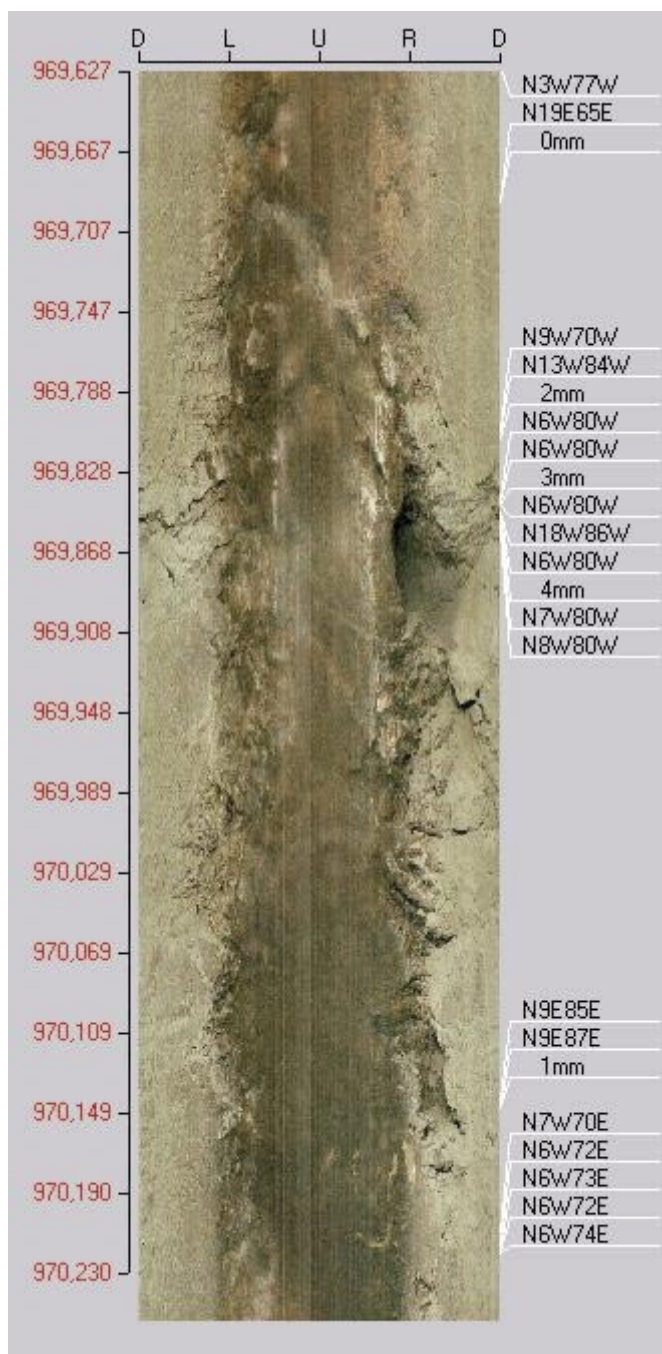


Figure A3-1. Borehole KFM07A: selected BIPS logging image from 969.6 to 970.2 m including the water bearing fractures /8/.

Measurement information, KFM07A

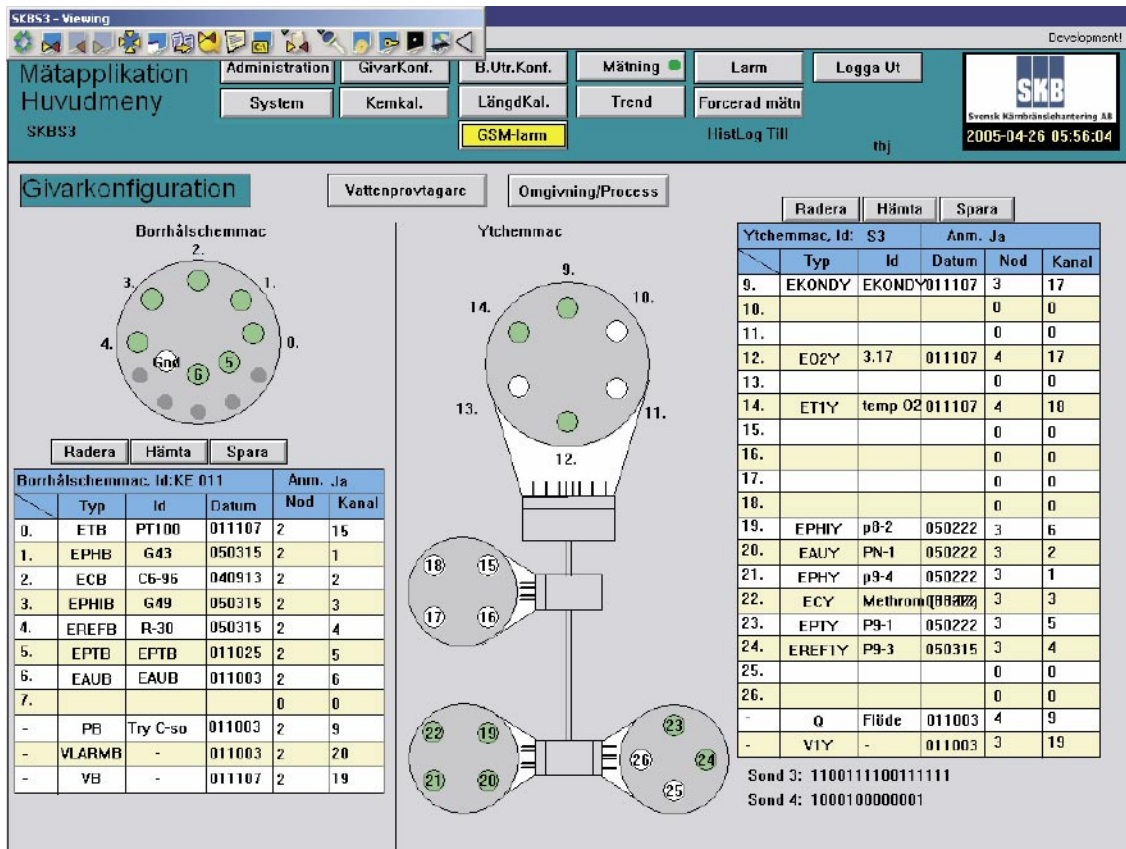


Figure A4-1. Electrode configuration, section 848.0–1,001.6 m.

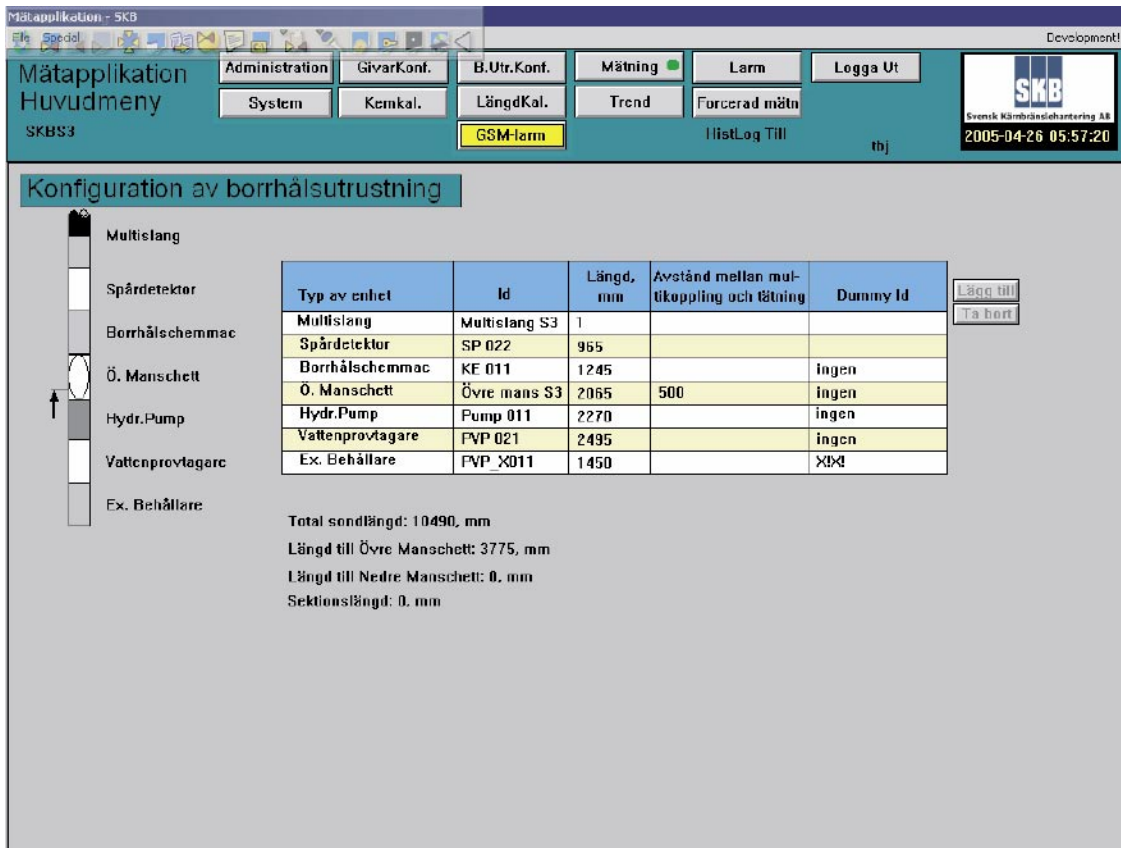


Figure A4-2. Configuration of downhole equipment, section 848.0–1,001.6 m.

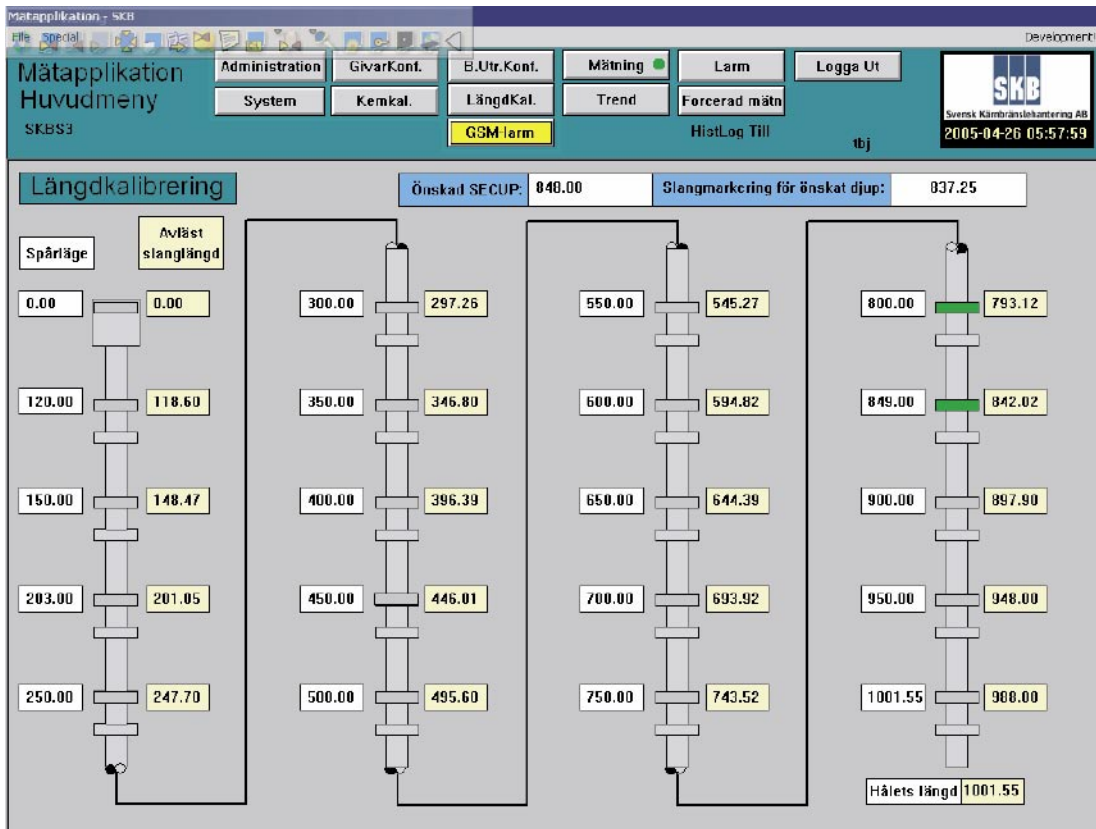


Figure A4-3. Length calibration, section 848.0–1,001.6 m.

Matapplikation - SKB

Administration | Givarkont. | B.Utr.Kont. | Mätning | Larm | Logga In

System | Kemkal. | LängdKal. | Trend | Forcerad mät. | GSM-larm | Hist. og Till

SKB
Svensk Kärnbränslehantering AB
2005-04-27 09:23:39

Administration

Utskrift

Export av mätfiler

Allmänt

Borrhål	KFM07a
Operatör	obj
SECUP	040.00
SECLOW	057.47
Starttid	2005-04-26 06:03:30
Stoptid	2005-04-26 14:35:16
Kemdata	KFM07a0426040K.MRB
OPData	KFM07a0426040K.MRB
Kommentar	KFM07a0426040K.ME
Filsbibliotek	D:\Mätfiler\KFM07a0503\0848-0857

Enhetsidentiteter

YChemmac	S3
Multislang	Multislang S3
Spår-detektor	SD 022
Borrhålschemmac	KE 011
Ö. Manöcher	Övre mans S3
Hydr.Pump	Pump 011
Vattenprovtagare	DVP 021
Ex. Behållare	PVP_X011

BorrhålsChemmac/PVP/OP

ETB	PT100
EPHB	G43
ECB	E6-96
EPHB	649
EREFB	R-30
EPTB	EPTB
EAUB	EAUB
PB	Try C-50
P1V	ePb
P2V	ePv
INTEMP	hw36
UTTEMP	ur78
ATMP	as7
GVNV	16.32334
RUMPP	v20823/13
MANSHIP	S03074/14

YChemmac

Q	Flöde
EKONDV	EKONDV
EOZY	3.17
ETLV	temp O2
EPHIV	p8-2
EAUV	PN-1
EPHV	p9-4
ECV	Methrem (05-02)
EDTV	p9-1
EREFIV	p9-3

CHEMMAC

		Filer - inkalibrering		Filer - utkalibrering	
		Data	Kommentar	Data	Kommentar
Y T	pH4	KFM07a03161pH4V.CRB	KFM07a03161pH4V.CI	KFM07a0426UpH4V.CRB	KFM07a0426UpH4V.CI
	pH7	KFM07a03161pH7V.CRB	KFM07a03161pH7V.CI	KFM07a0426UpH7V.CRB	KFM07a0426UpH7V.CI
	pH10	KFM07a03161pH10V.CRB	KFM07a03161pH10V.CI	KFM07a0426UpH10V.CRB	KFM07a0426UpH10V.CI
	0.01M	KFM07a03171kcl01V.CRB	KFM07a03171kcl01V.CI	KFM07a0426Ukcl01V.CRB	KFM07a0426Ukcl01V.CI
R O H Å R L	0.1M	KFM07a03171kcl1V.CRB	KFM07a03171kcl1V.CI	KFM07a0426Ukcl1V.CRB	KFM07a0426Ukcl1V.CI
	pH4	KFM07a03161pH4B.CRB	KFM07a03161pH4B.CI	KFM07a0426UpH4B.CRB	KFM07a0426UpH4B.CI
	pH7	KFM07a03161pH7B.CRB	KFM07a03161pH7B.CI	KFM07a0426UpH7B.CRB	KFM07a0426UpH7B.CI
	pH10	KFM07a03161pH10B.CRB	KFM07a03161pH10B.CI	KFM07a0426UpH10B.CRB	KFM07a0426UpH10B.CI

Figure A4-4. Administration, section 848.0–1,001.6 m.

Flow and pressure measurements in KFM07A

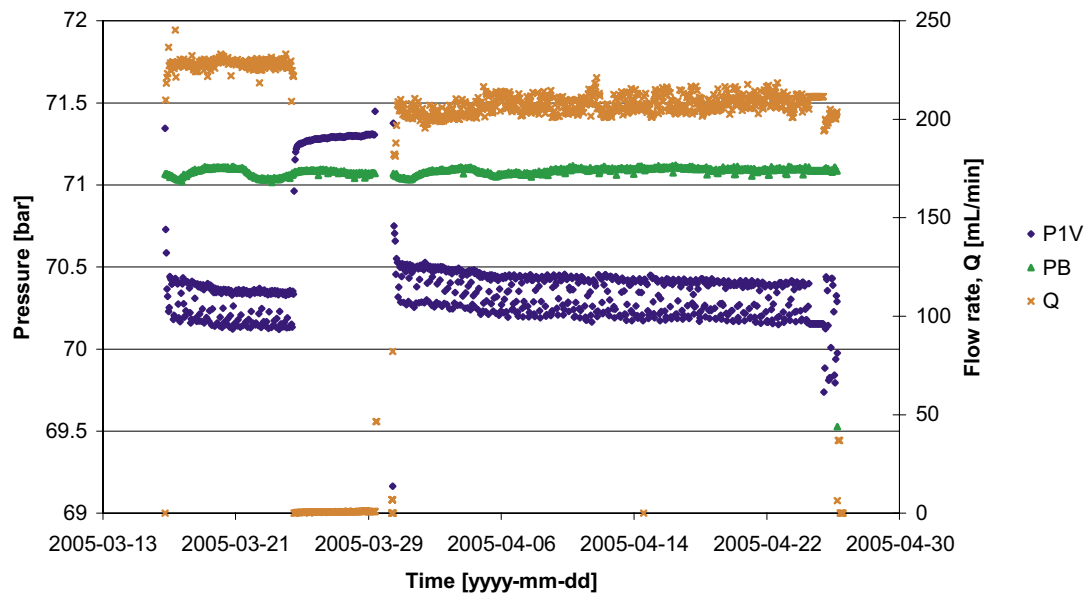


Figure A5-1. Pressure measured within the section (P1V) as well as above the section (PB) and pumping flow rate (Q), borehole section 848.0–1,001.6 m.

Chemmac measurements in KFM07A, section 848.0–1,001.6 m

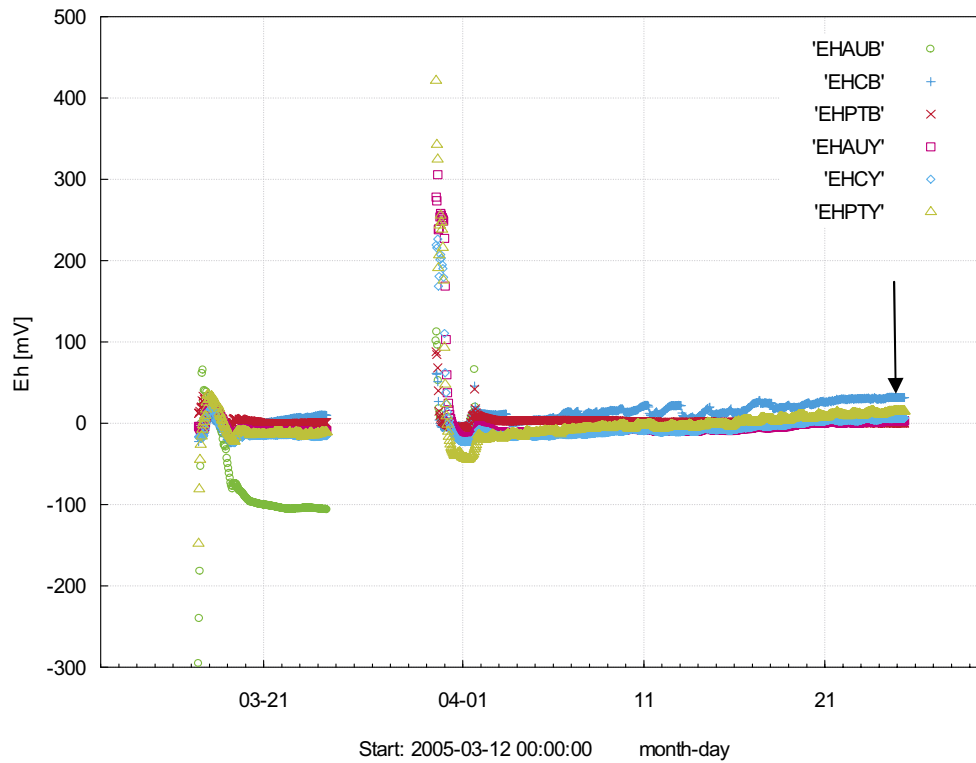


Figure A6-1. Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.

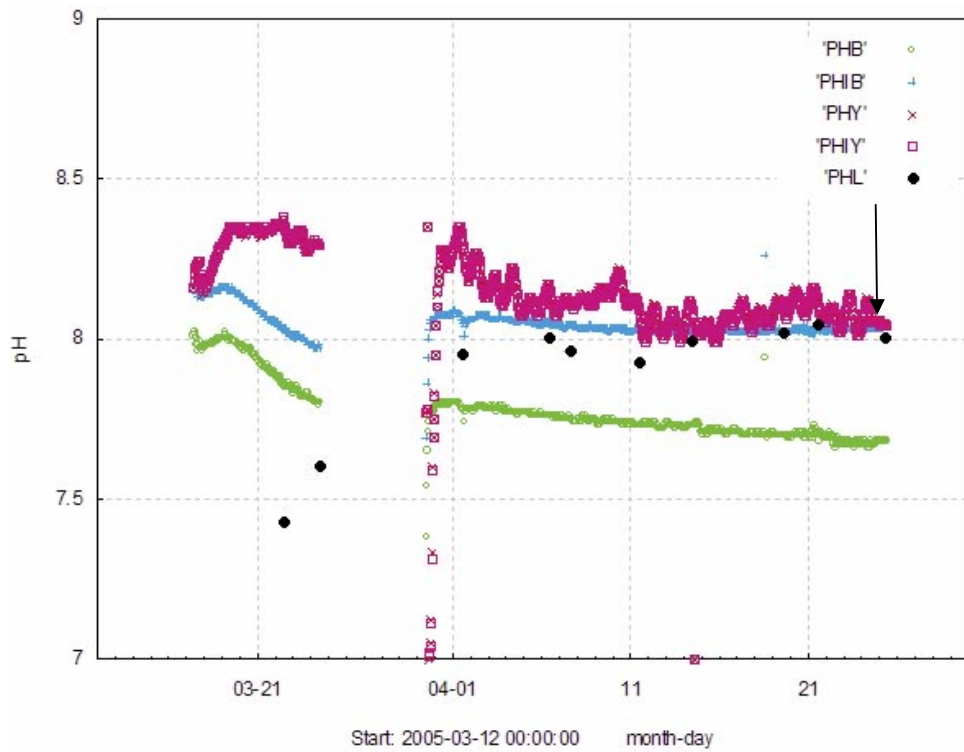


Figure A6-2. Measurements of pH by two glass electrodes in the borehole section (PHB and PHIB) and two glass electrodes at the surface (PHY and PHIY). The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values.

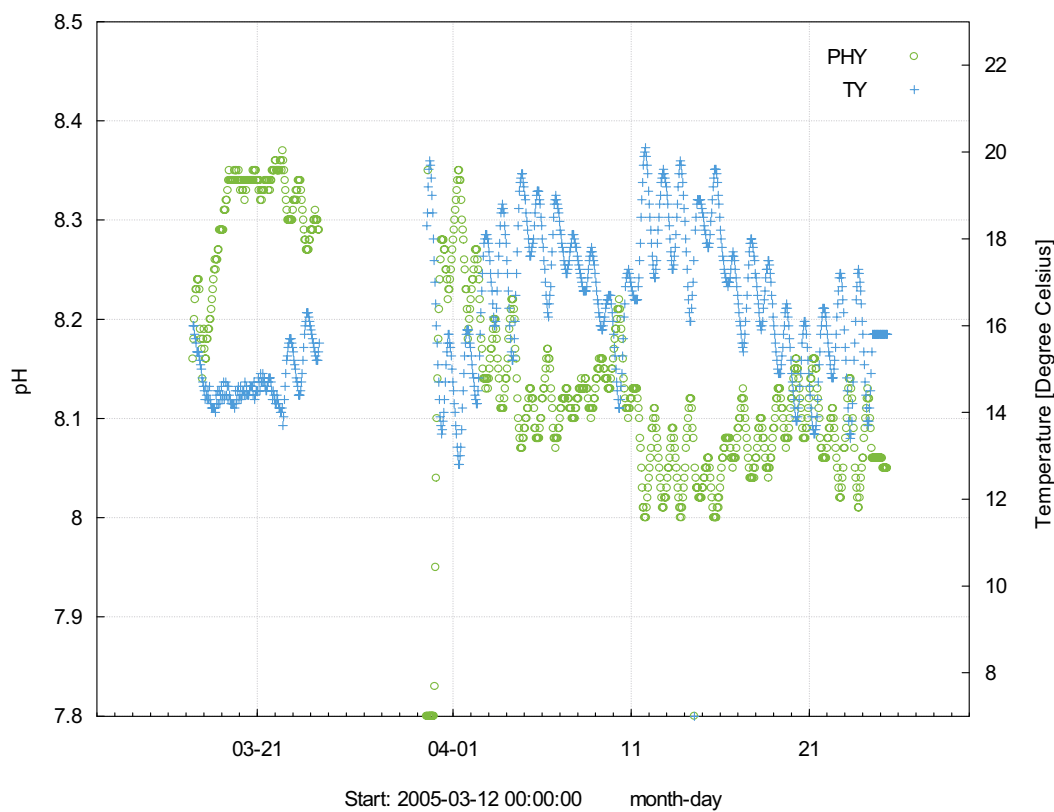


Figure A6-3. Measurements of pH by the two glass electrodes in the surface (PHY and PHIY) and the temperature at the surface (TY) show coherence, PHY are shown in the diagram.

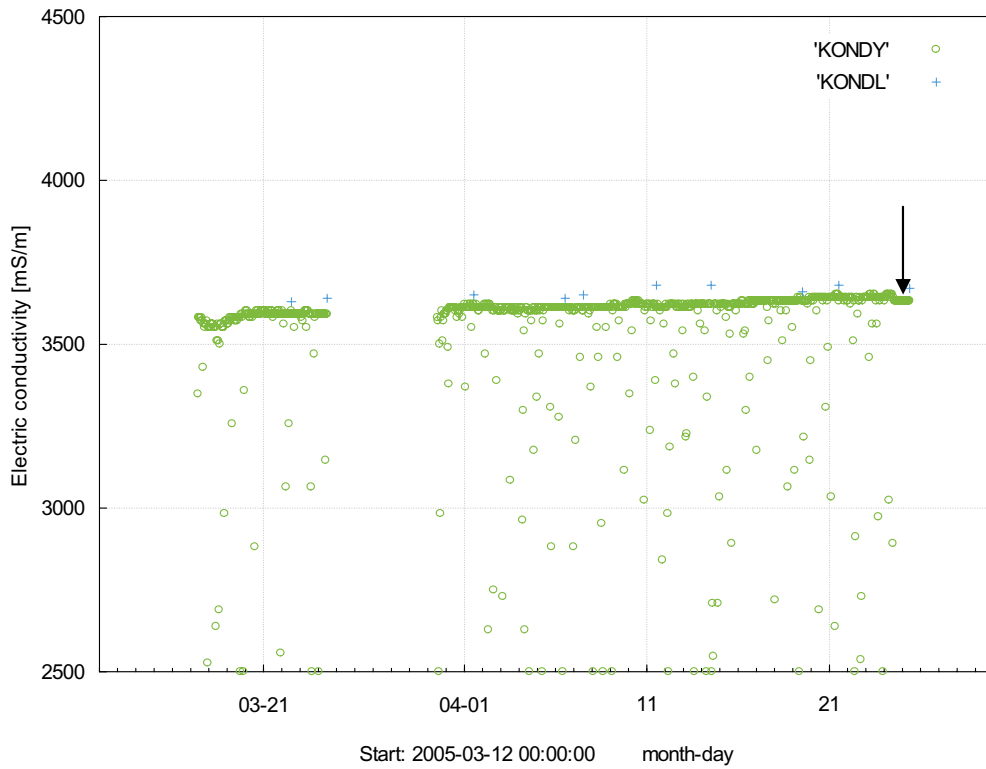


Figure A6-4. Electrical conductivity measurements in the surface measurement cell (KONDY). The laboratory conductivity in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative value for electrical conductivity.

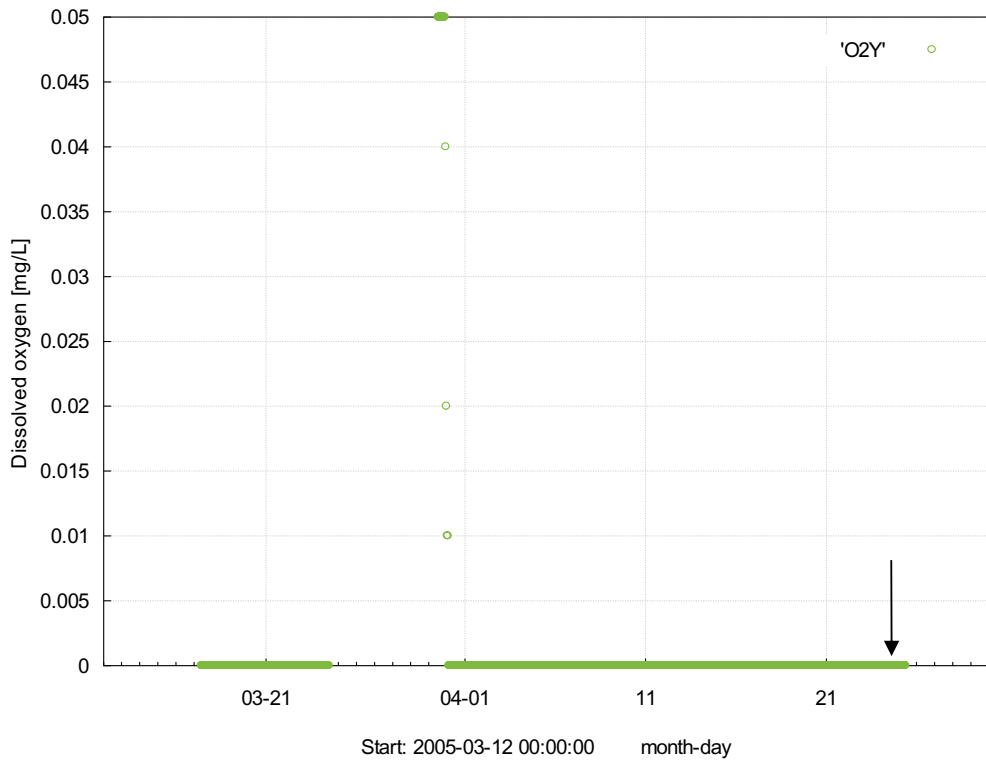


Figure A6-5. Dissolved oxygen measurements (O2Y) in the surface measurement cell. The arrow shows the chosen representative value for dissolved oxygen.

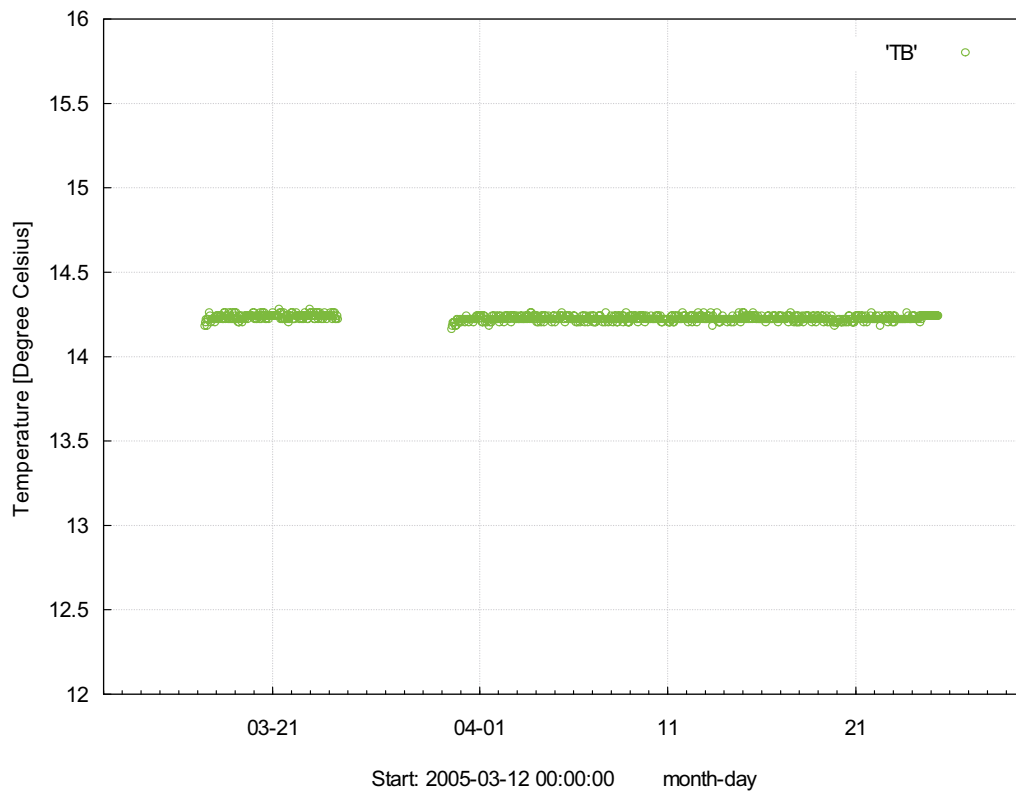


Figure A6-6. Temperature of the groundwater in the borehole section (TB).

Sampling and analysis methods

Table A7-1. Sample handling routines and analytical methods.

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.
Anions 1.	HCO ₃ , pH(lab), cond (lab)	Plastic	250	Yes (not in the field)	No	Titration Pot. meas, Cond. meas	The same day – maximum 24 hours
Anions 2	Cl, SO ₄ , Br ⁻ , F ⁻ , I ⁻	Plastic	100	Yes (not in the field)	No	Titration (Cl ⁻) IC (Cl ⁻ , SO ₄ , Br ⁻ , F ⁻) ISE (F ⁻)	Not critical (month)
	Br, I	Plastic	100	Yes (not in the field)	No	ICP MS	Not critical (month)
Cations, Si and S according to SKB class 3	Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr	Plastic (at low conc. acid washed bottles)	100	Yes (not in the field)	Yes (not in the field, 1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Cations, Si and S according to SKB class 4 and 5	Na, K, Ca, Mg, S(tot), Si(tot), Fe, Mn, Li, Sr	Plastic (Acid washed)	100	Yes (immediately in the field)	Yes (1mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic (Acid washed)	500	Yes	Yes (5 mL HCl)	Spectrophotometry Ferrozine method	As soon as possible the same day
Hydrogen sulphide	HS-	Glass (Winkler)	About 120×2	No	Ev 1 mL 1 M NaOH+ 1 mL 1M ZnAc	Spectrophotometry	Immediately or if conserved, a few days
Environmental metals	Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Lantanoids, U, Th and so on.	Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Dissolved organic Carbon, dissolved inorganic Carbon	DOC, DIC	Plastic	250 25	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.
Total organic Carbon	TOC	Plastic	250 25	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time
Environmental isotopes	² H, ¹⁸ O	Plastic	100	No	–	MS	Not critical (month)
Tritium,	³ H (enhanced.)	Plastic (dry bottle) Plastic	500	No	–	LSC	Not critical (month)
Chlorine-37	Chlorine-37		100	No	–	ICP MS	
Carbon isotopes	¹³ C, ¹⁴ C	Glass (brown)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	³⁴ S	Plastic	500–1,000	Yes	–	Combustion, ICP MS	No limit
Strontium-isotopes	⁸⁷ Sr/ ⁸⁶ Sr	Plastic	100	Yes	–	TIMS	Days or Week
Uranium and Thorium isotopes	²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th,	Plastic	50	Nej	–	Chemical separat. Alfa/gamma spectrometry	No limit
Boron isotopes	¹⁰ B	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP – MS	No limit
Radon and Radium isotopes	²²² Rn, ²²⁶ Ra	Plastic	500	No	No	EDA, RD-200	Immediate transport
Dissolved gas (content and composition)	Ar, N ₂ , CO ₂ , O ₂ , CH ₄ , H ₂ , CO, C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₈	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series and fractionation (see below)	Polycarbonate filter	0.45, 0.2 and 0.05 μm	–	N ₂ atmosphere	ICP-AES ICP-MS	Immediate transport
Humic and fulvic acids	Fractionation	Fractions are collected in plastic bottles	250	–	N ₂ atmosphere	UV oxidation, IR (DOC)	Immediate transport
Archive samples with acid	–	Plast (washed in acid)	100×2 **	Yes	Yes (1 mL HNO ₃)	–	Storage in freeze container
Archive samples without acid	–	Plastic	250×2 **	Yes	No	–	Storage in freeze container
Carbon isotopes in humic and fulvic acids	¹³ C, ¹⁴ C (pmc)	DEAE cellulose (anion exchanger)	–	–	–	(A)MS	A few days
Nutrient salt + silicate	NO ₂ , NO ₃ , NO ₂ +NO ₃ , NH ₄ , PO ₄ , SiO ₄	Sample tubes, plastic	25×2	Yes (in the field)	No, frozen immediately***	Spectrophotometry	Short transportation time
Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within – or delivery time to lab.

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.
Total concentrations of Nitrogen and Phosphorous	N-tot, P-tot	Plastic	100	No	No, frozen immediately***	Spectrophotometry	Short transportation time
Particulate Carbon, Nitrogen and Phosphorous	POC, PON, POP	Plastic	1,000	Yes (within 4 h) prepared filters. Blank filters	Filtering, the filters are frozen immediately 2 filters/sample	Elementar-analysator (N, C) own method 990121 (P)	Short transportation time
Chlorophyll	Chlorophyll a, c and pheopigment	Plastic	1,000–2,000	Yes (within 4 h)	Filtering, the filters are frozen immediately	Spectrophotometry Fluorometry	Short transportation time
Oxygen	Dissolved O ₂	Winkler, glass	2×ca 120	No	Mn (II) reagent Iodide reagent	Spectrophotometry SIS SS-EN 25813	Within 3 days
Archive samples for supplementary radio nuclides		Plastic	5,000	No	50 mL HNO ₃	–	Storage in freeze container

* Suprapur acid is used for conservation of samples.

** Minimum number. The number of archive samples can vary depending on the number of similar samples collected at the same occasion.

*** The sample is transported in frozen condition to the laboratory. It is possible that the silicate concentration can change due to polymerisation for this reason.

Abbreviations and definitions:

IC	Ion chromatograph
ISE	Ion selective electrode
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectrometry
ICP-MS	Inductively Coupled Plasma Mass Spectrometry
INAA	Instrumental Neutron Activation Analysis
MS	Mass Spectrometry
TIMS	Thermal Ionization Mass Spectrometer
LSC	Liquid Scintillation Counting
(A)MS	(Accelerator) Mass Spectrometry
GC	Gas Chromatography

Table A7-2. Reporting limits and measurement uncertainties.

Component	Method	Reporting limits or range	Unit	Measurement uncertainty ²	"Total" uncertainty ³
HCO ₃	Alkalinity titration	1	mg/L	4%	< 10%
Cl ⁻	Mohr- titration	> 70	mg/L	5%	< 10%
Cl ⁻	IC	1-100		6%	10%
SO ₄	IC	1	mg/L	10%	15%
Br ⁻	IC	0.2	mg/L	9%	20%
Br ⁻	ICP	0.001		15%	
F ⁻	IC	0.1	mg/L	10%	20%
F ⁻	Potentiometric	-		-	
I ⁻	ICP	0.001	mg/L	15%	20%
Na	ICP	0.1	mg/L	4%	10%
K	ICP	0.4	mg/L	6%	15%
Ca	ICP	0.1	mg/L	4%	10%
Mg	ICP	0.09	mg/L	4%	10%
S(tot)	ICP	0.160	mg/L	21%	15%
Si(tot)	ICP	0.03	mg/L	4%	15%
Sr	ICP	0.002	mg/L	4%	15%
Li	ICP	0.2 ¹ 2	mg/L	10%	20%
Fe	ICP	0.4 ¹ 4	mg/L	6%	10%
Mn	ICP	0.03 ¹ 0.1	µg/L	8%	10%
Fe(II), Fe(tot)	Spectrophotometry	0.02 (DL = 0.005 mg/L)	mg/L	15% (> 30 µg/L)	20%
HS ⁻	Spectrophotometry	SKB 0.03 (DL = 0.02)	mg/L	10%	30%
NO ₂ as N	Spectrophotometry	0.1	µg/L	2%	20%
NO ₃ as N	Spectrophotometry	0.2	µg/L	5%	20%
NO ₂ +NO ₃ as N	Spectrophotometry	0.2	µg/L	0.2 (0.2-20 µg/L) 2% (> 20 µg/L)	20%
NH ₄ as N	Spectrophotometry	0.8	µg/L	0.8 (0.8-20 µg/L) 5% (> 20 µg/L)	20%
		50 (SKB)		20%	
PO ₄ as P	Spectrophotometry	0.7	µg/L	0.7 (0.7-20 µg/L) 3% (> 20 µg/L)	20%
SiO ₄	Spectrophotometry	1	µg/L	3% (> 200 µg/L)	-
O ₂	Jodometric titration	0.2-20	mg/L	5%	-
Chlorophyll a, c pheopigment ⁴	See table A1-2	0.5	µg/L	5%	-
PON ⁴	See table A1-2	0.5	µg/L	5%	-
POP ⁴	See table A1-2	0.1	µg/L	5%	-
POC ⁴	See table A1-2	1	µg/L	4%	-
Tot-N ⁴	See table A1-2	10	µg/L	4%	-
Tot-P ⁴	See table A1-2	0.5	µg/L	6%	-
Al, Zn	ICP	0.2	µg/L	12%	20% ⁵
Ba, Cr, Mo, Pb	ICP	0.01	µg/L	7-10%	20% ⁵
Cd, Hg	ICP	0.002	µg/L	9 resp 5%	20% ⁵
Co, V	ICP	0.005	µg/L	8 resp 5%	20% ⁵
Cu	ICP	0.1	µg/L	8%	20% ⁵
Ni	ICP	0.05	µg/L	8%	20% ⁵
P	ICP	1	µg/L	6%	10%
As	ICP	0.01	µg/L	20%	Correct order of size(low conc)
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb	ICP	0.0051 0.05	µg/L	10%	Correct order of size (low conc)

Component	Method	Reporting limits or range		Unit	Measurement uncertainty ²	"Total" uncertainty ³
Sc, In, Th	ICP	0.05 ¹	0.5	µg/L	10%	Correct order of size (low conc)
Rb, Zr, Sb, Cs, Tl	ICP	0.025 ¹	0.25	µg/L	10%	Correct order of size (low conc)
Y, Hf	ICP	0.005 ¹	0.05	µg/L	10%	Correct order of size (low conc)
U	ICP	0.001 ¹	–	µg/L	12%	Correct order of size (low conc)
DOC	See table A1-1	0.5		mg/L	8%	30%
TOC	See table A1-1	0.1		mg/L	10%	30%
δ ² H	MS	2		‰ SMOW ⁵	1‰	–
δ ¹⁸ O	MS	0.1		‰ SMOW ⁵	0.2‰	–
³ H	LSC	0.8 eller 0.1		TU ⁶	0.8 eller 0.1	–
³⁷ Cl	ICP MS	0.2‰ (20 mg/L)		‰ SMOC ⁷	–	–
δ ¹³ C	A (MS)	–		‰ PDB ⁸	–	–
¹⁴ C pmc	A (MS)	–		PMC ⁹	–	–
δ ³⁴ S	ICP MS	0.2‰		‰ CDT ¹⁰	0.3‰	–
⁸⁷ Sr/ ⁸⁶ Sr	TIMS	–		No unit (ratio) ¹¹	–	–
¹⁰ B/ ¹¹ B	ICP MS	–		No unit (ratio) ¹¹	–	–
²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th	Alfa spectr.	0.0005		Bq/L ¹³	5%	–
²²² Rn, ²²⁶ Rn	LSC	0.03		Bq/L	5%	–

1. Reporting limits at salinity ≤ 0.4‰ (520 mS/m) and ≤ 3.5‰ (3,810 mS/m) respectively.

2. Measurement uncertainty reported by consulted laboratory, generally 95% confidence interval.

3. Estimated total uncertainty by experience (includes effects of sampling and sample handling).

4. Determined only in surface waters and near surface groundwater.

5. Per mille deviation¹³ from SMOW (Standard Mean Oceanic Water).

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

7. Per mille deviation¹³ from SMOC (Standard Mean Oceanic Chloride).

8. Per mille deviation¹³ from PDB (the standard PeeDee Belemnite).

9. 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.

10. Per mille deviation¹³ from CDT (the standard Canyon Diablo Troilite).

11. Isotope ratio without unit.

12. The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232:

$$1 \text{ ppm U} = 12.4 \text{ Bq/kg}^{238}\text{U}$$

$$1 \text{ ppm Th} = 3.93 \text{ Bq/kg}^{232}\text{Th}$$

13. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:

$$\delta\text{‰} = 1,000 \times (K_{\text{sample}} - K_{\text{standard}}) / K_{\text{standard}}, \text{ where } K = \text{the isotope ratio and } \text{‰} = {}^2\text{H}, {}^{18}\text{O}, {}^{37}\text{Cl}, {}^{13}\text{C} \text{ or } {}^{34}\text{S} \text{ etc.}$$

Compilation of water analysis data

Table A8-1. Water composition, compilation of basic water analysis data.

Idcode	Secup m	Seclow m	Sample no	Sampling date	Charge Bal%	Na mg/L	K mg/L	Ca mg/L	Mg mg/L	HCO ³⁻ mg/L	Cl ⁻ mg/L	SO ₄ ²⁻ mg/L	SO ₄ -S mg/L	Br mg/l	F ⁻ mg/L	Si mg/L	Fe mg/L	Fe-tot mg/L	Fell mg/L
KFM07A	848.00	1,001.55	8842	2005-03-22	1.3	2,810	17.6	5,760	21.7	7.99	14,100	98.0	36.5	198	1.36	4.64	0.314	0.320	0.304
KFM07A	848.00	1,001.55	8843	2005-03-24	-0.0	2,780	13.5	5,740	21.5	7.36	14,400	103	36.3	196	1.36	4.73	0.277	0.288	0.262
KFM07A	848.00	1,001.55	8844	2005-04-01	0.3	2,830	17.0	5,810	21.5	7.24	14,500	97.2	36.1	212	1.31	4.57	0.424	0.327	0.310
KFM07A	848.00	1,001.55	8865	2005-04-06	0.3	2,820	16.1	5,810	21.4	6.59	14,500	101	36.3	203	1.36	4.81	0.248	0.245	0.226
KFM07A	848.00	1,001.55	8866	2005-04-07	-0.5	2,830	13.6	5,780	21.1	7.56	14,700	99.5	35.8	176	1.35	4.72	0.210	0.249	0.234
KFM07A	848.00	1,001.55	8875	2005-04-11	0.2	2,820	15.7	5,740	20.9	9.38	14,400	97.9	35.6	200	1.36	4.80	0.225	0.227	0.203
KFM07A	848.00	1,001.55	8876	2005-04-14	0.0	2,830	13.2	5,760	20.7	6.59	14,500	96.6	36.4	192	1.30	4.84	0.208	0.227	0.208
KFM07A	848.00	1,001.55	8877	2005-04-19	0.3	2,900	14.5	5,800	20.0	6.37	14,600	98.2	36.5	210	1.42	4.90	< 0.2	0.188	0.166
KFM07A	848.00	1,001.55	8878	2005-04-21	0.2	2,810	13.4	5,810	20.3	6.45	14,500	102	36.5	198	1.30	4.89	< 0.2	0.178	0.170
KFM07A	848.00	1,001.55	8879	2005-04-25	-0.4	2,850	13.7	5,840	19.9	6.19	14,800	99.3	36.4	186	1.34	4.85	0.196	0.188	0.162

Cont Table A8-1. Water composition, compilation of basic water analysis data.

Idcode	Secup m	Seclow m	Sample no	Sampling date	Mn mg/L	Li mg/L	Sr mg/L	I ⁻ mg/L	pH	DOC mg/L	HS ⁻ mg/L	Drill_water %	EiCond mS/m	NH ₄ N mg/L
KFM07A	848.00	1,001.55	8842	2005-03-22	0.145	0.072	69.2	-	7.43	1.8	0.134	0.40	3,630	0.0273
KFM07A	848.00	1,001.55	8843	2005-03-24	0.141	0.074	68.4	0.748	7.60	2.0	0.080	0.60	3,640	0.0189
KFM07A	848.00	1,001.55	8844	2005-04-01	0.144	0.072	66.1	-	7.95	< 1	0.185	0.65	3,650	0.020
KFM07A	848.00	1,001.55	8865	2005-04-06	0.138	0.080	69.3	-	8.00	< 1	0.133	0.40	3,640	0.013
KFM07A	848.00	1,001.55	8866	2005-04-07	0.137	0.072	69.8	0.689	7.96	< 1	0.104	0.35	3,650	0.0161
KFM07A	848.00	1,001.55	8875	2005-04-11	0.135	0.076	70.5	-	7.93	< 1	0.255	0.25	3,680	0.0163
KFM07A	848.00	1,001.55	8876	2005-04-14	0.133	0.076	69.4	0.740	7.99	< 1	0.093	0.40	3,680	0.010
KFM07A	848.00	1,001.55	8877	2005-04-19	0.131	0.065	68.8	-	8.02	< 1	0.106	0.20	3,660	0.0142
KFM07A	848.00	1,001.55	8878	2005-04-21	0.130	0.075	69.6	0.777	8.04	< 1	0.098	0.65	3,680	0.0112
KFM07A	848.00	1,001.55	8879	2005-04-25	0.127	0.096	69.5	0.721	8.00	< 1	0.171	0.35	3,670	0.0183

Table A8-2. Compilation of H-, O-, B-, S-, Cl- and C-isotopes and isotope ratios.

Idcode	Secup m	Seclow m	Sample no	Sampling date	$\delta^2\text{H}$ ‰ SMOW	^3H TU	$\delta^{18}\text{O}$ ‰ SMOW	$^{10}\text{B}/^{11}\text{B}$ no unit	$\delta^{34}\text{S}$ ‰ CDT	$\delta^{13}\text{C}$ ‰ PDB	$^{87}\text{Sr}/^{86}\text{Sr}$ no unit	^{14}C pmC	$\delta^{37}\text{Cl}$ ‰ SMOC
KFM07A	848.00	1,001.55	8842	2005-03-22	-90.0	< 0.8	-12.94	0.2399	-	-	-	-	-
KFM07A	848.00	1,001.55	8843	2005-03-24	-87.1	< 0.8	-12.90	0.24	22.8	-	0.717855	-	0.01
KFM07A	848.00	1,001.55	8844	2005-04-01	-89.6	< 0.8	-13.0	0.2390	-	-	-	-	-
KFM07A	848.00	1,001.55	8865	2005-04-06	-87.0	< 0.8	-13.0	0.2396	-	-	-	-	-
KFM07A	848.00	1,001.55	8866	2005-04-07	-87.0	< 0.8	-13.0	0.24	24.7	-	0.717909	-	0.33
KFM07A	848.00	1,001.55	8875	2005-04-11	-87.2	< 0.8	-13.0	0.2407	-	-	-	-	-
KFM07A	848.00	1,001.55	8876	2005-04-14	-86.6	< 0.8	-13.0	0.2387	25.0	-	0.717911	-	-
KFM07A	848.00	1,001.55	8877	2005-04-19	-86.2	< 0.8	-13.0	0.24	-	-	-	-	0.07
KFM07A	848.00	1,001.55	8878	2005-04-21	-86.3	-	-13.1	0.2371	25.2	-	0.717915	-	0.16
KFM07A	848.00	1,001.55	8879	2005-04-25	-86.7	-	-13.1	0.2386	30.2	A	0.717914	A	0.08

Table A8-3. Compilation of trace elements.

Idcode	Secup m	Seclow m	Sample no	Sampling date	U µg/L	Th µg/L	Al µg/L	Sc µg/L	Rb µg/L	Y µg/L	Zr µg/L	In µg/L	Sb µg/L	Cs µg/L	La µg/L	Hf µg/L	Tl µg/L	Ce µg/L	Pr µg/L	Nd µg/L
KFM07A	848.00	1,001.55	8843	2005-03-24	0.337	< 0.4	-	1.47	46.6	0.817	< 0.6	< 1	0.981	1.00	< 0.1	< 0.1	< 0.6	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8866	2005-04-07	0.323	< 0.4	-	1.15	43.4	0.747	< 0.6	< 1	0.941	1.00	< 0.1	< 0.1	< 0.6	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8876	2005-04-14	0.28	< 0.4	-	1.03	44	0.727	< 0.6	< 1	0.900	1.00	< 0.1	< 0.1	< 0.6	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8878	2005-04-21	0.264	< 0.4	-	1.19	46.6	0.806	< 0.6	< 1	0.864	1.09	< 0.1	< 0.1	< 0.6	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8879	2005-04-25	0.184	< 0.4	3.75	< 1	44.1	0.78	< 0.6	< 1	1.330	1.03	< 0.1	< 0.1	< 0.6	< 0.1	< 0.1	< 0.1

Cont Table A8-3. Compilation of trace elements.

Idcode	Secup m	Seclow m	Sample no	Sampling date	Sm µg/L	Eu µg/L	Gd µg/L	Tb µg/L	Dy µg/L	Ho µg/L	Er µg/L	Tm µg/L	Yb µg/L	Lu µg/L
KFM07A	848.00	1,001.55	8843	2005-03-24	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8866	2005-04-07	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8876	2005-04-14	< 0.1	0.103	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8878	2005-04-21	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1
KFM07A	848.00	1,001.55	8879	2005-04-25	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1

Table A8-4. Compilation of U-, Th-, Ra- and Rn-isotope data.

Idcode	Secup m	Seclow m	Sample no	Sampling date	²³⁸ U mBq/L	²³⁵ U mBq/L	²³⁴ U mBq/L	²³² Th mBq/L	²³⁰ Th mBq/L	²²⁶ Ra Bq/L	²²² Rn Bq/L
KFM07A	848.00	1,001.55	8879	2005-04-25	A	A	A	A	A	14.5	138

Table A8-5. Dissolved gases.

Idcode	Secup m	Seclow m	Sample no	Sampling date	Ar mL/L	He mL/L	N ₂ mL/L	CO ₂ mL/L	CH ₄ mL/L	O ₂ mL/L	H ₂ µL/L	CO µL/L	C ₂ H ₆ µL/L	C ₂ H ₄ µL/L	C ₂ H ₂ µL/L	C ₃ H ₈ µL/L	C ₃ H ₆ µL/L	DISS_GAS mL/L H ₂ O
KFM07A	848.00	1,001.55	8879	2005-04-26	1.7	26	133	< 4.8	0.040	0.19	< 4.8	< 8.0	0.66	< 0.08	< 0.08	< 0.16	< 0.16	161