P-06-08

Oskarshamn site investigation

Complete chemical characterisation in KLX03

Results from four investigated borehole sections: 193.5–198.4 m, 408.0–415.3 m, 735.5–748.0 m, 964.5–975.2 m

Anette Bergelin, Cecilia Berg, Pia Wacker
Geosigma AB

December 2006

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

ISSN 1651-4416
SKB P-06-08

Oskarshamn site investigation

Complete chemical characterisation in KLX03

Results from four investigated borehole sections: 193.5–198.4 m, 408.0–415.3 m, 735.5–748.0 m, 964.5–975.2 m

Anette Bergelin, Cecilia Berg, Pia Wacker
Geosigma AB

December 2006

Keywords: Groundwater, Measurements on line, In situ sampling, Measurements in situ, Redox potential, Dissolved gas, Humic and fulvic acids, Colloids, Microbes, Chemical analyses, Isotope determinations, Hydrochemical characterisation, KLX03, Site investigation, AP PS 400-04-042.

Abstract

Complete chemical characterisation has been conducted in four sections 193.5–198.3, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m of borehole KLX03. This 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 during approximately three weeks per section at a flow rate of between 50 and 200 mL/min.

The results obtained from the *Complete chemical characterisation* of sections 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m 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. In section 735.5–748.0 m, there was no investigation of humic and fulvic acids due to high amounts of remaining flushing water (> 10%).

The water composition was stable during the entire pumping and sampling periods in sections 193.5–198.4 and 964.5–975.2 m. In section 408.0–415.3 m the composition seem to stabilise at the end of the pumping period and in section 735.5–748.0 m there was an increase in the composition of major constituents during the entire sampling period. The chloride concentrations were approximately 260 mg/L (193.5–198.4 m), 1,000–1,400 mg/L (408.0–415.3 m), 2,800–4,000 mg/L (735.5–748.0 m) and 10,500 mg/L (964.5–975.2 m).

Stable redox potential measurements are reported for the three sections 193.5–198.4, 408.0–415.3 and 735.5–748.0 m. The redox electrodes stabilised at approximately –285,–271 and –210 mV respectively. The reducing conditions in the groundwater of these sections were also verified by the presence of ferrous iron Fe(+II) at relatively high concentrations. In section 964.5–975.2 m, the redox electrodes did not reach stable and credible values within the measurement period. This is probably due to the very low iron concentration in the groundwater of this section and thereby a lack of a dominating redox pair.

The content of inorganic colloids in the water was very low or nonexistent with respect to silicon and manganese. The presence of colloidal aluminium and iron is uncertain since contamination and precipitation have to be considered.

The organic constituents were present mainly as fulvic acids and possibly other low molecular weight organic acids (citric acid, oxalic acid, etc) in the deepest section (964.5–975.2 m). There appears to be a fraction of organic constituents with larger molecular weight in sections 193.5–198.4 m and 408.0–415.3 m.

Sammanfattning

Fullständig kemikarakterisering har utförts i de fyra borrhålssektionerna 193.5–198.4, 408.0–415.3, 735.5–748.0 och 964.5–975.2 m av borrhålet KLX03. Metoden är den mest omfattande kemiska undersökningsmetoden för kärnborrhål. Den innebär pumpning, mätning on-line och regelbunden vattenprovtagning för kemiska analyser i avgränsade borrhålssektioner under cirka tre veckor per sektion och vid ett pumpflöde på mellan 50 och 200 mL/min.

Resultaten som erhölls från den fullständiga kemikarakteriseringen av sektionerna 193.5–198.4, 408.0–415.3, 735.5–748.0 och 964.5–975.2 m omfattar mätningar on-line av redoxpotential, pH, löst syre, elektrisk konduktivitet och vattentemperatur i borrhålssektionen liksom kemiska analyser av huvudkomponenter, spårelement och isotoper. Vidare undersöktes gasmängd och sammansättning, oorganiska kolloider samt humus- och fulvosyror i grundvattnet. I sektion 735.5–748.0 m undersöktes inte humus- och fulvosyror på grund av hög spolvattenhalt (> 10 %).

Vattensammansättningen var stabil under hela pump- och provtagningsperioderna i borrhålssektionerna 193.5–198.4 och 964.5–975.2 m. I sektion 408.0–415.3 m verkade sammansättningen stabiliseras i slutet av pumpperioden och i sektion 735.5–748.0 m kunde en ökande trend noteras under hela provtagningsperioden. Kloridkoncentrationerna uppgick till cirka 260 mg/L (193.5–198.4 m), 1 000–1 400 mg/L (408.0–415.3 m), 2 800–4 000 mg/L (735.5–748.0 m) och 10 500 mg/L (964.5–975.2 m).

Stabila redoxpotentialer rapporteras för de tre sektionerna 193.5–198.4, 408.0–415.3 och 735.5–748.0 m. Redoxelektroderna stabiliserade sig vid cirka –285, –271 respektive –210 mV. De reducerande förhållandena i grundvattnet i dessa sektioner verifieras också av närvaron av tvåvärt järn i relativt höga koncentrationer. I sektionen 964.5–975.2 m nådde inte redoxelektroderna stabila och trovärdiga värden under mätperioden. Detta beror förmodligen på de mycket låga järnkoncentrationerna i grundvattnet i denna sektion och därmed avsaknad av ett dominerande redoxpar.

Förekomsten av oorganiska kolloider befanns vara mycket låg eller obefintlig vad gäller kisel och mangan. Förekomsten av kolloidalt aluminium och järn är osäker då kontaminering och utfällning kan påverka resultatet.

De organiska komponenterna förelåg huvudsakligen som fulvosyror eller andra lågmolekylära organiska syror (citronsyra, oxalsyra) i den lägsta sektionen (964.5–975.2 m). I sektionerna 193.5–198.4 och 408.0–415.3 m observerades även en fraktion av organiska komponenter med högre molekylär vikt.

Contents

1 Introduction

This document reports performance of and results from the activity *Complete hydrochemical characterisation* in the cored borehole KLX03 performed within the site investigation at Oskarshamn /1/. The work was conducted according to the activity plan AP PS 400-04-042 (SKB internal controlling document). The controlling documents for the performance of this activity are listed in Table 1-1. Both activity plan and method descriptions are SKB internal controlling documents). The data obtained is reported to the database SICADA and traceable from the activity plan numbers.

The report presents hydrochemical data from the following five borehole sections:

- 193.5–198.4 metres.
- 408.0–415.3 metres.
- 660.0–670.7 metres; interrupted investigation, limited amounts of data.
- 735.5–748.0 metres.
- 964.5–975.2 metres.

The field work was carried out during the period November 2004–April 2005. Sampling for microbe studies, based on activity plan AP PS 400-04-042 (SKB internal controlling document), was also performed within the present activity. The microbe investigations are presented in a separate primary data report /2/.

Borehole KLX03 is a 1,000.4 m long telescopic borehole drilled at Laxemar and inclined 75° from the horizontal direction. The interval 0–100 m is percussion drilled with a diameter of 200 mm and the interval 100–1,000.4 m is core drilled with a diameter of 76 mm. The percussion borehole HLX14 served as the source of flushing water for the drilling of KLX03. The locations of KLX03 and HLX14 are shown in Figure 1-1. The borehole design of KLX03 is presented in Appendix 1.

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

Activity plan	Number	Version
Fullständig kemikaraktärisering med mobilt fältlaboratorium i KLX03.	AP PS 400-04-042	1.0
Method descriptions	**Number**	**Version**
Metodbeskrivning för fullständig kemikaraktärisering med mobilt fältlaboratorium.	SKB MD 430.017	1.0
Mätsystembeskrivning för kolloidfiltreringssystem	SKB MD 431.045	In progress
Mätsystembeskrivning för uppkoncentrering av humus- och fulvosyror.	SKB MD 431.044	1.0
Mätsystembeskrivning för fraktionering av humus- och fulvosyror.	SKB MD 431.043	1.0
Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning.	SKB MD 600.004	1.0

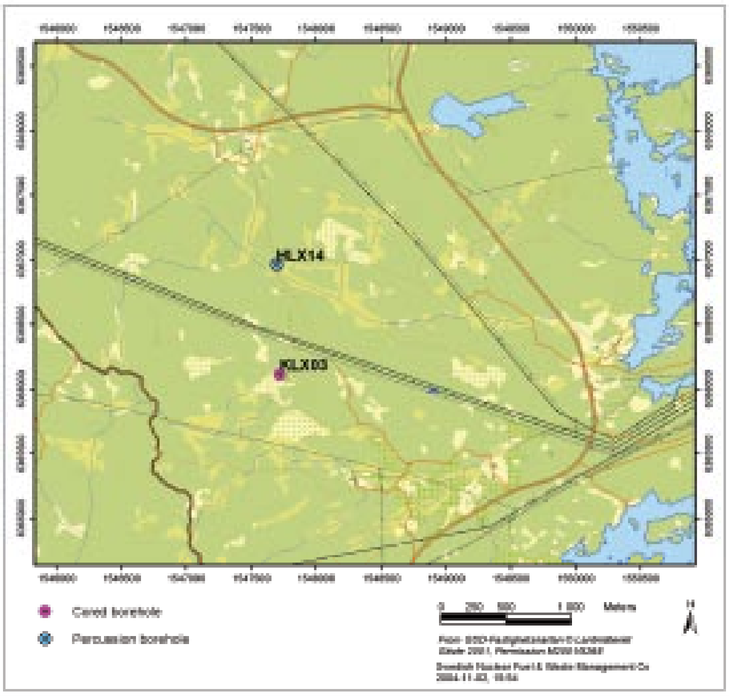


Figure 1-1. *Locations of the core drilled borehole KLX03 and the supply well HLX14 within the site investigation at Oskarshamn.*

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

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 obtain as complete information as possible about the groundwater chemical conditions in individual water bearing fractures or local minor fracture zones. Considerable effort is made to obtain 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.

The analytical programme is carried out according to SKB chemistry class 4 and class 5 including all options. In addition pH, redox potential (Eh) and water temperature are measured in downhole flow-through cells in the pumped borehole section as well as at the ground surface. The flow-through cell at the surface also measures electrical conductivity and dissolved oxygen. The investigation also includes in situ samples in the borehole section for determination of gas content and composition, microbe content and their characterisation as well as colloid investigation. Moreover, fractionation of organic acids and inorganic species are performed to investigate size distribution (DOC and metal ions). Enrichment of organic acids is conducted in order to determine $\partial^{13}C$ and pmC (percent modern carbon).

3 Background

3.1 Previous activities in the borehole

KLX03 is a SKB chemistry-type core borehole intended for *Complete chemical characterisation*. Only activities that are necessary in order to choose borehole sections are carried out in the borehole prior to the chemistry campaign. The more equipment that is used in the borehole, the greater is the risk of contamination and effects on the in situ microbiological conditions. The activities performed in KLX03 after completed core drilling and prior to the *Complete chemical characterisation* are listed in Table 3-1 below.

Table 3-1. Activities performed in borehole KLX03 prior to the *Complete chemical characterisation.*

Activity	Date of completion	Length or section (m)	Comment
Hydrochemical logging	2004-09-21	990	/3/
BIPS-logging	2004-09-26	100–994,180	/4/
Geophysical logging	2004-10-26	100–1,000	/5/
Difference flow logging	2004-11-17	101.30–992.37	/6/

4 Equipment

4.1 The mobile field laboratory

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, Figure 4-1; the system is presented schematically in Figure 4-2. 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 (Mätsystembeskrivningar för mobil kemienhet allmän del, slangvagn, borrhålsutrustning, mobil ytChemmac och dataapplikation).

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

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

The mobile units used in borehole KLX03 consisted of the hose unit S2 and the laboratory unit L2 and the MYC 2 unit for computer work. The equipment used for colloid filtration, enrichment of humic and fulvic acids and fractionation of humic and fulvic acids are described below.

***Figure 4-1.** The mobile units at KLX03; from left container for collecting the water from the borehole, laboratory unit, hose unit with downhole equipment and a unit for computer work, January 2005.*

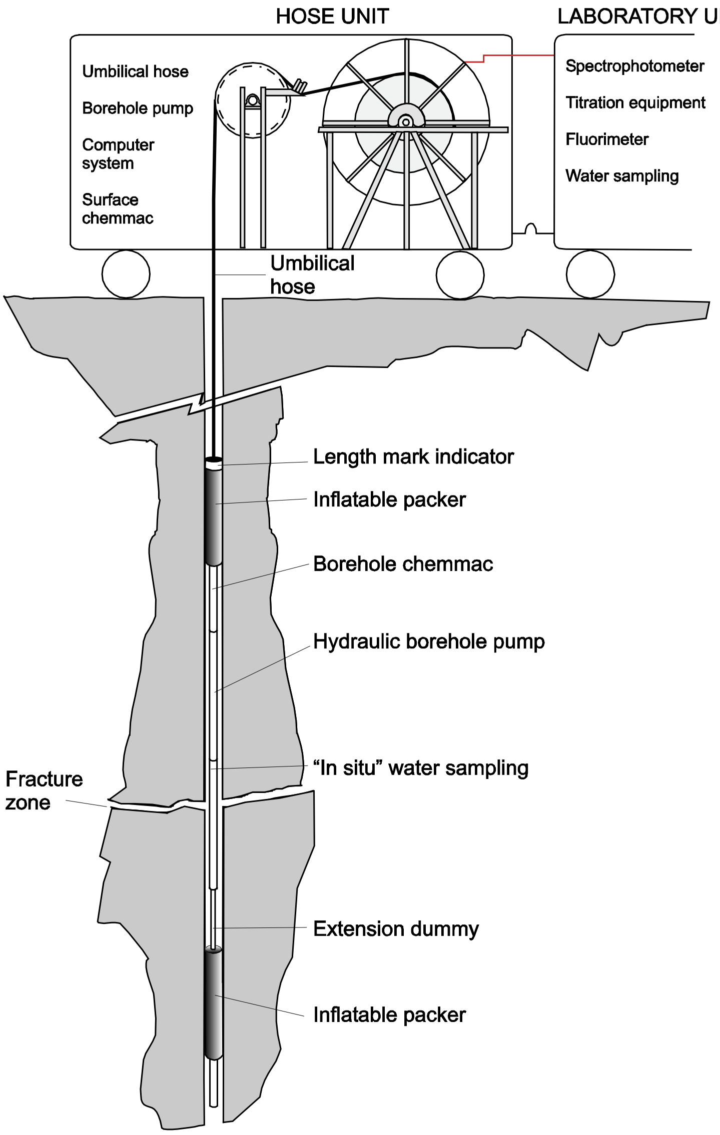


Figure 4-2. *The mobile laboratory including laboratory unit, hose unit and downhole equipment. The configuration of the downhole units in the borehole can be varied depending on desired section length. However, the in situ water sampler must always be positioned first in the sample water path.*

4.2 Colloid filtering equipment

The equipment is adapted to the sample containers (PVB) from the PVP water sampling unit. The colloid filtering equipment 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 (Mätsystembeskrivning för kolloidfiltreringssystem, handhavandedel (SKB internal controlling document to be published)). Figure 4-3 shows the equipment.

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.

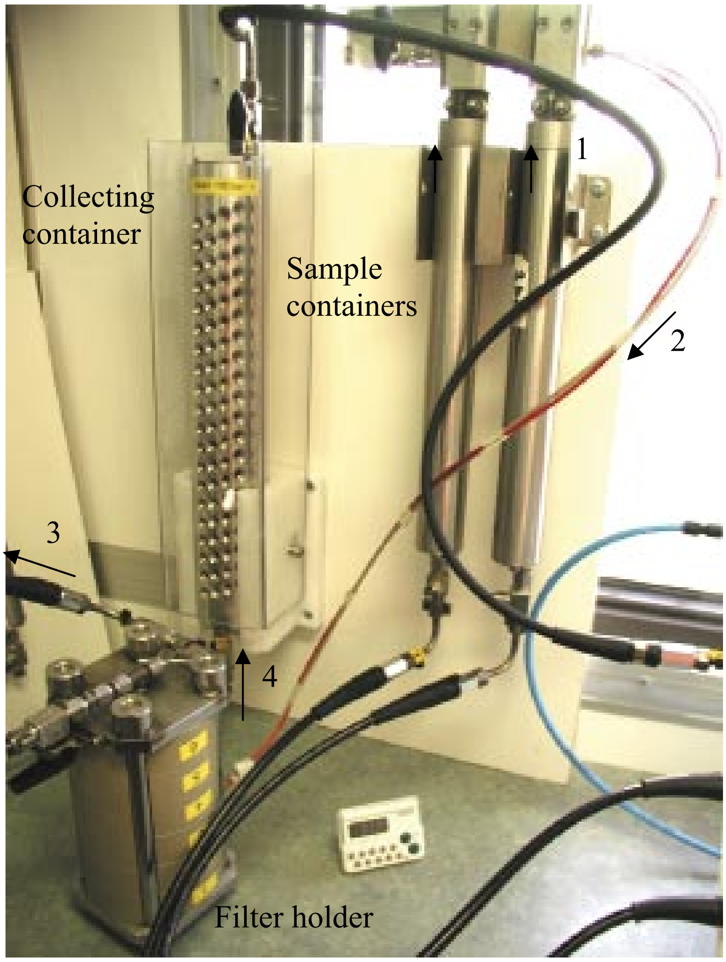


Figure 4-3. *The colloid filtering equipment including the sample containers, the filter holder package and the collecting container. The black arrows, 1 to 4, show the flow direction of the sample water through the system.*

- The design of the sample containers, and the mounting with the outlet at the top, prevents migration of larger particles that may clog the filters. Furthermore, clogging is prevented by the first two filters with pore sizes 0.4 µm which are mounted parallel to each other.

Disadvantages/drawbacks that may cause modifications of 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. If the method proves to be successful, an improvement could be to use Teflon coating on the insides of the cylindrical containers.

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 $\partial^{13}C$ 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 4-4

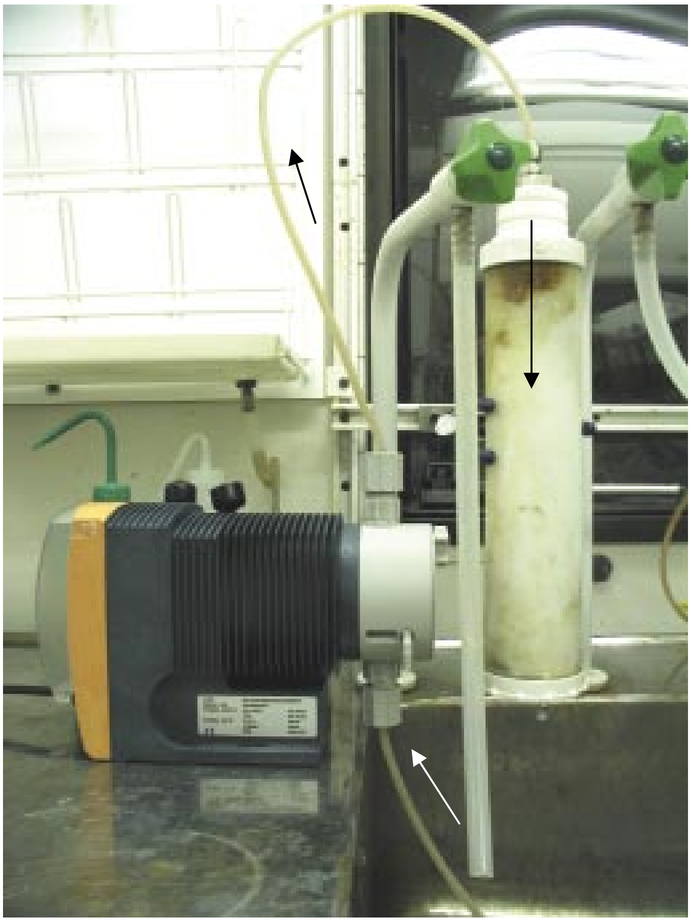


Figure 4-4. *The ion exchange column. The arrows show the water flow direction.*

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 was used for pumping a portion of the outlet water through the column (approximately 2.4 L/hour).

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, one water sample 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 (Mätsystembeskrivning för fraktionering av humus- och fulvosyror, SKB internal controlling document). Figure 4-5 shows the equipment setup.

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

5 Performance

5.1 General

Chemical characterisation of the six sections in borehole KLX03 was performed according to the activity plan and following the methods descriptions.

An overview of the investigation sequence and pumped volume during the chemical characterisation is given in Table 5-1.

During the period 2004-12-21 to 2005-01-17 "Clean up" pumping was performed by SKB in order to decrease the flushing water content. The pump was lowered to a depth of 20 m down the borehole and the total pumped volume was approximately 200 m^3.

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 and 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.

Table 5-1. Investigation sequence and pumped volume during the chemical characterisation in KLX03.

Start date/stop date	Section (m)	Pumped volume
2004-11-25/2004-12-16	193.5–198.4	6.6 m^3
2005-01-18/2005-01-21	660.0–670.7	1.0 m^3 Interrupted investigation.
2005-01-21/2005-02-15	964.5–975.2	7.6 m^3
2005-02-18/2005-03-22	408.0–415.3	7.1 m^3
2005-03-22/2005-04-26	735.5–748.0	8.0 m^3

The different downhole units are assembled during lowering of the equipment in 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, a length mark detector unit (caliper) is mounted together with the downhole equipment. The length mark detector indicates length calibration marks milled into the borehole wall at almost every 50 m along the borehole. 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 since the greater the drawdown, the larger the bedrock volume affected by the pumping and the risk of mixing with water from other fracture systems increases. The pumping flow rate is adjusted depending on the flow yield from the fracture or fracture zone (to between 50 and 300 mL/min) 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 and pH measurements and by immediate analyses (chloride, alkalinity, ammonium, ferrous and total iron).
- 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 ∂^{13}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 suitable 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 193.5–198.4 m

The investigation carried out in borehole section 193.5–198.4 m was performed with the following configuration of the downhole equipment, starting from the top: umbilical hose, length mark detector, borehole Chemmac, borehole pump, upper packer, in situ water sampler (PVP) and lower packer, see Appendix 3. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping was performed at a flow rate of about 230 mL/min. A diagram showing the pressures above and within the section and the flow rate during the pumping/measurement period is presented in Appendix 4, Figure A4-1.

The events during the investigation are listed in Table 5-2.

Table 5-2. Events during the pumping/measurement period in section 193.5–198.4 m.

Date	Events *Improvement/deviation*	SKB sample no.
041124	Calibration of borehole Chemmac.	
041125	**Lowering of downhole equipment (193.50–198.37 m).**	
	Start of Chemmac measurements.	
	The electrical distributor was broken during lowering. Needed to be repaired before lifting.	
	A higher pressure is needed to run the pump, at the surface, to achieve high flow with the new umbilical hose. Before 35 bar and an engine frequency of 38% was needed, now a pressure of approximately 60 bar and a frequency of 70% are used to attain the same flow.	
041126	Calibration of surface Chemmac.	
	Water sampling: pH, electrical conductivity, alkalinity, chloride and Uranine.	7946
041129	Water sampling: SKB class 4.	7947
041201	Water sampling: SKB class 5.	7948
	Humic and fulvic acids; enrichment start.	
041203	Water sampling: SKB class 4.	7949
041206	Water sampling: SKB class 5.	7950
041209	Water sampling: SKB class 4.	7951
041213	Water sampling: SKB class 5.	7952
041214	Humic and fulvic acids; fractionation 1 kD.	7953
041215	Humic and fulvic acids; fractionation 5 kD.	7953
	Water sampling: SKB class 5 including density.	7953
	Water sampling: SKB class 5. Control sample.	7954
	PVP-sampler: opening of valve at 15:04.	
041216	Humic and fulvic acids; enrichment stop.	
	PVP-sampler: closure of valve at 08:07.	
	End of Chemmac measurements.	
	Lifting.	
	Sampling of microbes and dissolved gases.	7953
	Sampling of colloids.	
	Colloid filtration.	7953
	Calibration of borehole Chemmac.	
041217	Calibration of surface Chemmac.	
	The file KLX031125193K.MI is missing. Could not be restored.	
041220	Humic and fulvic acids; enrichment eluation.	7953

5.4 Performance in section 408.0–415.3 m

The investigation carried out in section 408.0–415.3 m was performed with the following configuration of the downhole equipment, starting from the top: umbilical hose, length mark detector, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP) and lower packer, see Appendix 3. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping was performed at a flow rate of about 170–240 mL/min. A diagram showing the pressures above and within the borehole section and the flow rate during the pumping/measurement period is presented in Appendix 4, Figure A4-2.

The events during the investigation are listed in Table 5-3.

5.5 Performance in section 660.0–670.7 m

The investigation carried out in section 660.0–670.7 m was performed with the following configuration of the downhole equipment, starting from the top: umbilical hose, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP), extension dummy and lower packer.

The pumping was performed at a flow rate of about 230–260 mL/min.

The events are listed in Table 5-4.

Table 5-3. Events during the pumping/measurement period in section 408.0–415.3 m.

Date	Events *Improvement/deviation*	SKB sample no.
050216	Calibration of surface Chemmac.	
	Power failure.	
050217	Calibration of borehole Chemmac after power failure.	
	Lowering of downhole equipment (408.00–415.30 m).	
	Leakage at swivel connection into the drum at the umbilical hose. O-rings and ring laps are replaced.	
050218	**Start of Chemmac measurements.**	
	Water sampling: pH, electrical conductivity, alkalinity and Uranine.	10082
050221	Water sampling: SKB class 4.	10083
050223	Water sampling: Uranine.	10084
	Humic and fulvic acids; enrichment start.	
050224	Water sampling: SKB class 5.	10085
050228	Water sampling: SKB class 4.	10086
050307	*The water level in the tank providing the packers with water has decreased. The problem is caused by a leakage in a thread at the lower packer.*	
050308	**Lifting.**	
050309	Calibration borehole Chemmac	
	Lowering of downhole equipment (408.00–415.30 m).	
	Calibration surface Chemmac	

Date	Events *Improvement/deviation*	SKB sample no.
050310	*Leakage at a de-air plug to the packers in the coupling to the umbilical hose. Caused by a defect o-ring.*	
	Lifting.	
	Lowering of downhole equipment (408.00–415.30 m).	
	The pressure gauge in the chemical probe KE021 out of order. Ceased to function during lifting.	
	Water sampling: Uranine.	10087
050311	Water sampling: SKB class 4.	10088
050314	Water sampling: SKB class 4.	10089
050317	Water sampling: SKB class 5.	10090
	Humic and fulvic acids; fractionation 1 kD.	10091
050318	Humic and fulvic acids; fractionation 5 kD.	10091
050322	Water sampling: SKB class 5 including density.	10091
	Water sampling: SKB class 5. Control sample.	10183
	Humic and fulvic acids; enrichment stop.	
	PVP-sampler: opening of valve at 05:57.	
	PVP-sampler: closure of valve at 06:46.	
	End of Chemmac measurements.	
	Lifting.	
	Sampling of microbes and dissolved gases.	10091
	Sampling of colloids.	
	Colloid filtration.	10091
	Humic and fulvic acids; enrichment eluation.	10091
	Calibration of borehole Chemmac.	
050323	Calibration of surface Chemmac.	

Table 5-4. Events during the pumping/measurement period in section 660.0–670.7 m.

Date	Events *Improvement/deviation*	SKB sample no.
050114	*Power failure due to hard weather (storm).*	
	Electrical power station QA18 is out of function. One of the phases drop out from time to time and causes equipment malfunction. Change of circuit breaker.	
	Malfunction in chemical probe KE021, two channels, 2 and 6. The electrodes show poor inclination and the responses from them are not satisfactory.	
050117	*Change of probe in hose unit (from KE021 to KE022). New probe does not measure the temperature correctly.*	
	Calibration of borehole Chemmac.	
050118	**Lowering of downhole equipment (660.00–670.65 m).**	
	Start of Chemmac measurements.	
050119	Calibration of surface Chemmac.	
	Water sampling: pH, electrical conductivity, alkalinity, chloride and Uranine.	10002
050120	Water sampling: Uranine.	10003
050121	Water sampling: Uranine.	10004
	Ending investigation in section due to high flushing water content. (Lowering of downhole equipment to the section at 964.5–975.2 m)	
	The GSM alarm in MYC2 is out of order.	

5.6 Performance in section 735.5–748.0 m

The investigation carried out in section 735.5–748.0 m was performed with the following configuration of the downhole equipment, starting from the top: umbilical hose, length mark detector, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP), extension dummy and lower packer, see Appendix 3. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping was performed at a flow rate of about 170–260 mL/min. A diagram showing the pressures above and within the borehole section and the flow rate during the pumping/measurement period is presented in Appendix 4, Figure A4-3.

The events during the investigation are listed in Table 5-5.

Table 5-5. Events during the pumping/measurement period in section 735.5–748.0 m.

Date	Events *Improvement/deviation*	SKB sample no.
050322	Calibration of borehole Chemmac.	
	Lowering of downhole equipment (735.50–748.04 m).	
	Start of Chemmac measurements.	
050323	*Poor contact with Chemmac probe.*	
	Lifting.	
	Searching for faults in coupling to umbilical hose.	
	Lowering of downhole equipment (735.50–748.04 m).	
	Calibration of surface Chemmac.	
	Water sampling: Uranine.	10184
050324	Water sampling: pH, electrical conductivity, alkalinity, chloride and Uranine.	10185
050326	*The automatic contact breaker released – no measurement values 050326–050328.*	
050329	Water sampling: SKB class 4 (analysis of pH, electric conductivity, Uranine, HCO_3^-, F^-, Br^-, Cl^-, SO_4^{2-}, Fe^{2+}, Fe_{tot}, HS^-, NH^+_4 and Tritium, the rest are stored in a freezer).	10186
	High power consumption, indicates lost contact with chemical probes in the borehole.	
	Lifting.	
050330	Calibration of borehole Chemmac.	
	Lowering of downhole equipment (735.50–748.04 m).	
050331	Water sampling: Uranine.	10187
	Temporary stop of borehole pump while disconnecting leaking swivel connection.	
	Calibration surface Chemmac.	
050401	Water sampling: SKB class 4.	10188
050404	Water sampling: SKB class 4.	10189
050405	Water sampling: Uranine.	10190
050407	Water sampling: SKB class 4.	10191
050408	Water sampling: Uranine.	10192
050411	*Broken spring in borehole pump.*	
	Lifting.	
	Lowering of downhole equipment (735.50–748.04 m).	
	Neither spring nor piston in delivered borehole pump.	
	Membrane in oxygen meter broken. Probably due to sudden pressure change when one of the electrodes loosened. Membrane replaced and oxygen meter calibrated.	
050412	**Lifting.**	
	Lowering of downhole equipment (735.50–748.04 m).	
	High power consumption, indicates lost contact. **Lifting.**	
050413	**Lowering of downhole equipment (735.50–748.04 m).**	
050414	Water sampling: Uranine.	10193

Date	**Events** ***Improvement/deviation***	**SKB sample no.**
050415	Water sampling: SKB class 5, Ra- and Rn-isotopes excluded.	10194
050418	Water sampling: SKB class 4.	10239
050419	Water sampling: Uranine.	10240
	Increasing redox potential values and oxygen level in the surface Chemmac, possibly caused by a defective oxygen meter. A leakage from the swivel is also observed.	
050420	*Membrane in oxygen meter replaced, oxygen meter calibrated.*	
050421	Water sampling: SKB class 5.	10241
050424	*Still no change in oxygen levels measured by the surface Chemmac. Membrane in oxygen meter replaced again. While replacing the oxygen meter an electrode loosen from the Chemmac. The surface Chemmac is unplugged until lifting, i.e. no surface Chemmac values are available.*	
050425	Water sampling: SKB class 5, including density.	10242
	Water sampling: SKB class 5. Control sample.	10243
050426	PVP-sampler: opening of valve at 05:46.	
	PVP-sampler: closure of valve at 06:46.	
	End of Chemmac measurements.	
	Lifting.	
	Sampling of microbes and dissolved gases.	10242
	Sampling of colloids.	
	Colloid filtration.	10242
	Calibration of borehole Chemmac.	
	Calibration of surface Chemmac.	

5.7 Performance in section 964.5–975.2 m

The investigation carried out in section 964.5–975.2 m was performed with the following configuration of the downhole equipment, starting from the top: umbilical hose, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP), extension dummy and lower packer, see Appendix 3. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping was performed at a flow rate of about 220–280 mL/min. A diagram showing the pressures above and within the borehole section and the flow rate during the pumping/measurement period is presented in Appendix 4, Figure A4-4.

The events during the investigation are listed in Table 5-6.

Table 5-6. Events during the pumping/measurement period in section 964.5–975.2 m.

Date	**Events** ***Improvement/deviation***	**SKB sample no.**
050117	Calibration of borehole Chemmac.	
050119	Calibration of surface Chemmac.	
050121	**Lowering of downhole equipment (964.50–975.15 m).**	
	Start of Chemmac measurements.	
050124	Water sampling: pH, electrical conductivity, alkalinity, chloride and Uranine.	10005
050125	Humic and fulvic acids; enrichment start.	
	Water sampling: SKB class 4.	10006
050127	Water sampling: SKB class 5.	10007
050129	*No flow from the section due to broken spring in borehole pump.*	
050202	**Lifting.**	

Date	Events *Improvement/deviation*	SKB sample no.
	Steer wheel scrapes against the chain guard to the extent that shavings occur and spark formations arises. The chain guard is modified to avoid future problems.	
	Lowering of downhole equipment (964.50–975.15 m).	
050203	Water sampling: Uranine.	10008
050204	Water sampling: SKB class 5, Ra- and Rn-isotopes excluded.	10009
050207	Water sampling: SKB class 4.	10074
	Water is leaking from the control valve at the pump, at the surface. Change of valve will be performed after lifting.	
050210	Humic and fulvic acids; fractionation 5 kD.	10076
	Humic and fulvic acids; fractionation 1 kD.	10076
	Water sampling: SKB class 5. Missing data; B^{10}, As, In, environmental metals, lantanoids and trace elements (rare earth metals and others).	10075
050214	Humic and fulvic acids; enrichment stop.	
	Water sampling: SKB class 5, including density.	10076
	Water sampling: SKB class 5. Control sample.	10077
050215	PVP-sampler: opening of valve at 06:58.	
	PVP-sampler: closure of valve at 08:03.	
	End of Chemmac measurements.	
	Lifting.	
	Sampling of microbes and dissolved gases.	10076
	Sampling of colloids.	
	Colloid filtration.	10076
	Humic and fulvic acids; enrichment eluation.	10076
	Calibration of borehole Chemmac.	
050216	Calibration of surface Chemmac.	

5.8 Water sampling, sample treatment and analyses

The pumped water from the borehole section is conveyed from the hose unit into the laboratory unit where sampling and sample filtration is carried out. Filtration of sample portions is performed on-line by connecting the filter holders directly to the water outlet. A water sample is defined as water 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 9. The routines are applicable independently of sampling method or type of sampling object.

One of the bottles with archive sample, from the control samples 7954, 10183, 10243 and 10077, were sent to Analytica (2005-10-03) for control analyses of Br^-. The results from the analyses are reported in Appendix 10. The results from the laboratory at Äspö were cancelled due to problems with the analyses.

5.9 Collection of in situ water samples

The in situ water sampling was conducted successfully in all four sections: 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m.

The PVB-containers were all controlled before use; this procedure includes de-assembling of the container, thorough cleaning, re-assembling and measurement of piston friction.

The purpose of each sample portion is given in Table 5-7.

Table 5-7. Collection and purpose of in situ water sample portions.

Sample portion no.	Section 193.5–198.4 m 2004-12-16	Section 408.0–415.3 m 2005-03-22	Section 735.5–748.0 m 2005-04-26	Section 964.5–975.2 m 2005-02-15
1	Dissolved gas	Dissolved gas	Dissolved gas	Dissolved gas
2	Microbes	Microbes	Microbes	Microbes
3	Colloid filtration	Colloid filtration	Colloid filtration	Colloid filtration
4	Colloid filtration	Colloid filtration	Colloid filtration	Colloid filtration

The two PVB-containers for colloid filtration were filtered the same day at the site. The PVB-containers for dissolved gases and microbes 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 day.

5.10 Colloid filtration

Colloid filtration was performed in all investigated sections, 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m respectively. The method for sampling of 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. Two of the four sample portions collected in situ in each borehole section are used for colloid filtration. Data on performance of the filtration runs are given in Table 5-8.

A leak test of the system at 10 bars was also done prior to the sampling in order to eliminate the risk of leakage. If no leakage was detected, the system was dried and assembled.

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).

Table 5-8. 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
193.5–198.4 m/ 20041216	~ 21	3.4	~ 9	119	272.4	Leakage test prior to filtration. No leakage was noticed.
408.0–415.3 m/ 20050322	~ 40	3.6	~ 11	60	303.0	Leakage test prior to filtration. No leakage was noticed.
735.5–748.0 m/ 20050426	~ 71.5	3.4	~ 16	29	334.5	Leakage test prior to filtration. No leakage was noticed.
964.5–975.2 m/ 20050215	~ 92	5.7 (the diff. pressure was increased from about 3 bars half way through the filtration in order to get the water through the filters)	~ 16	100	336.5	Leakage test prior to filtration. No leakage was noticed.

5.11 Enrichment of humic and fulvic acids

Enrichment of humic and fulvic acids was conducted in order to collect enough material to determine $\partial^{13}C$ and pmC in organic constituents in the groundwater. The enrichment method entails collection of organic acids on an ion exchanger, eluation of the resin and evaporation of the resulting solution. The method is described in SKB MD 431.044 (Mätsystembeskrivning för uppkoncentrering av humus- och fulvosyror). The dry residue is used for isotope determination; a minimum amount of 10 mg organic carbon is needed. 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 5-9. The enrichment was cancelled in section 735.5–748.0 m due to the high content of remaining flushing water (> 10%).

5.12 Fractionation of humic and fulvic acids

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

Fractionation of humic and fulvic acids took place in three out of four investigated sections i.e. in section 193.5–198.4, 408.0–415.3 and 964.5–975.2 m. In section 735.5–748.0, the fractionation was excluded due to the high content of remaining flushing water content (above 10%). Sampled water from the investigated sections 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 and common trace metals. The analyses of metal ions should indicate if metals such as Al, Si, Mn and Fe exist as colloidal species.

Table 5-9. Estimations of time and volume of water passing through the ion exchanger.

Borehole section (m)	Duration of enrichment (days)	Volume through ion exchanger (L)
193.5–198.4	12	543
408.0–415.3	17	623
964.5–975.2	15	670

6 Nonconformities

The *Complete chemical characterisation* of the four investigated sections in KLX03 has been conducted according to the SKB internal controlling documents for the activity. Some equipment malfunctions (listed in Tables 5-2 to 5-6) have occurred during the pumping/measurement periods.

- The investigation in section 660.0–670.7 m was interrupted after a few days. The section had high content of remaining flushing water (13%), no decreasing trend was shown. During an electrical power failure (stop of borehole pump), it was decided to interrupt the measurement.
- The temperature in section 964.5–975.2 m was not measured due to a defective temperature meter in the borehole Chemmac.
- Due to equipment malfunction the pressure above the investigated section, PB, was not measured at the end of the investigation in section 408.0–415.3 m and not at all in section 735.5–748.0 m.
- The allowed upper limit for flushing water content (1%) was exceeded in two sections i.e. section 408.0–415.3 m (2%) and section 735.5–748.0 m (11%); this is not reported in deviation reports.
- Control sample for analyses of Na, K, Ca, Mg, Si, Fe, Mn, Li, Sr and S-tot were excluded in section 735.5–748.0 m due to the high flushing water content (> 10%).
- The enrichment and fractionation activities of humic and fulvic acids were excluded in section 735.5–748.0 m due to the high flushing water content (> 10%).
- In section 408.0–415.3 and 735.5–748.0 m, problems with the postal service occurred during the shipment of samples no. 10083, 10085–10086, 10088–10091 and 10186, 10188, 10189, 10191, 10194, 10239, respectively, to the laboratory in Waterloo. This caused all analyses for carbon isotopes to be cancelled. The samples no. 10085, 10090, 10091 and 10194 were stored in refrigerator. The bottles with sample no. and the following analysis were lost during the shipment; 10085 for δ^{37}Cl, 10091 for both tritium and δ^{37}C and sample no. 10189 and 10194 for tritium. Tritium for sample no. 10194 was analysed from the same bottle as δ^{37}Cl. For section 408.0–415.3 m, the lost bottles and bottles for carbon isotopes were replaced by sending the control sample bottles from sample no. 10183 for analysis of tritium, δ^{37}Cl and carbon isotopes.

7 Data handling and interpretation

7.1 Chemmac measurement data

The processing of Chemmac data are described in SKB MD 434.007-02 (Mätsystembeskrivning 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 field work and the calculation/evaluation. The comments in the file are imported as activity comments in SICADA.

7.1.2 Calculations and evaluation of pH and redox potential

The redox potential is measured by three electrodes at the surface and three in the borehole section. In addition, pH is measured by two electrodes at the surface and two 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 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.

Some 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 ± 5% are considered acceptable (in surface waters ± 10%).

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

- 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.

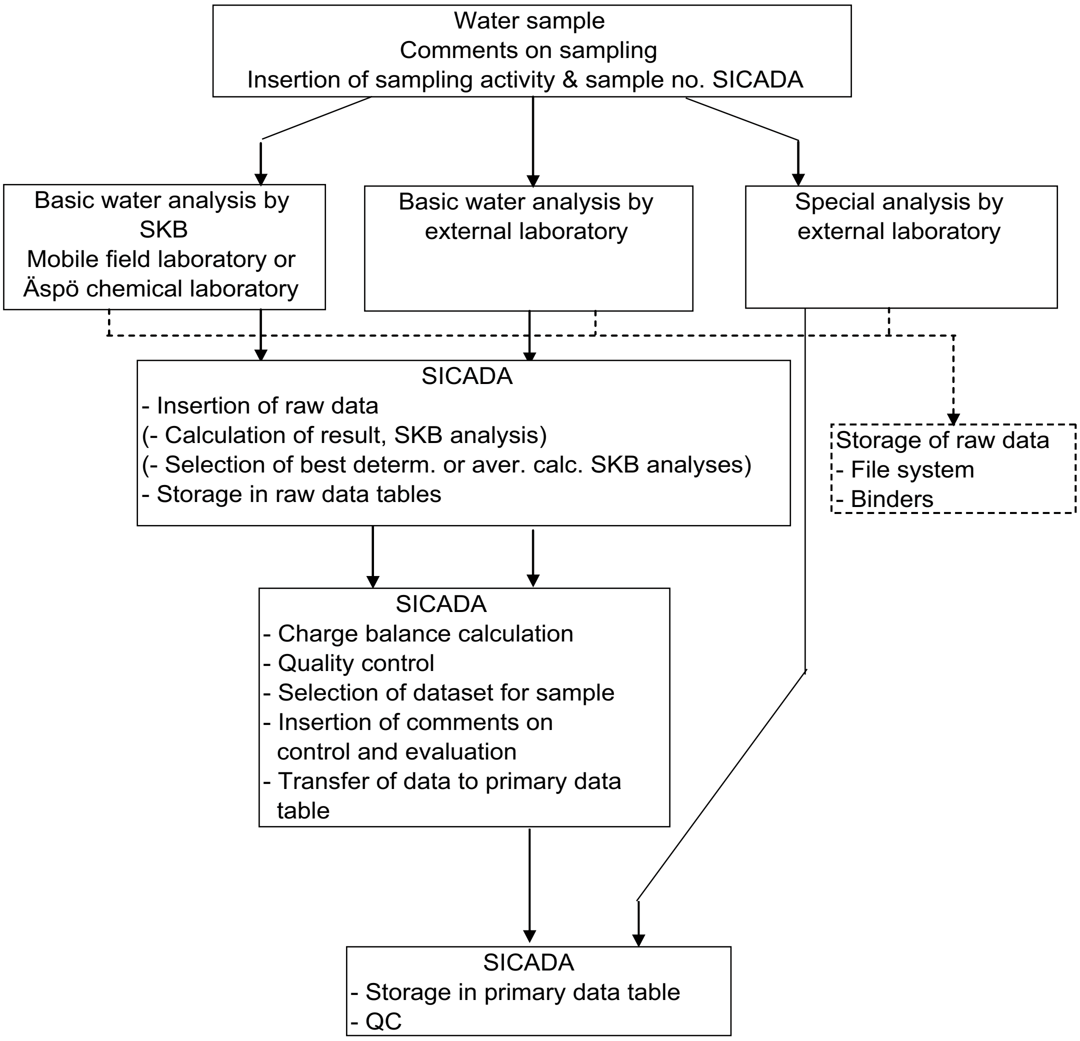


Figure 7-1. Overview of data management for hydrogeochemical data.

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 ∂^{13}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 colloid 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 calculated results from the colloid filtration, filters, are stored in SICADA. The water samples (in and outgoing water) are directly inserted into the primary data tables 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 δ^{13}C 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 re-calculated 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, (Mätsystembeskrivning för fraktionering av humus- och fulvosyror, SKB internal controlling document). 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 redox potentials in sections 193.5–198.4, 408.0–415.3 and 735.5–748.0 m were stable and negative. However, the surface electrodes in sections 193.5–198.4 and 735.5–748.0 m gave positive redox potentials. A reason for this could be intrusion of oxygen. The redox electrodes in section 964.5–975.2 m did not reach a stable potential within the measurement period. This is probably due to the low iron concentration in the groundwater and thereby lacks of a dominating redox pair. The potential from the carbon electrode was considered the most reliable since it is generally so that the true potential is lower than the measured. The pH given by the borehole electrodes was lower than the pH given by those in the surface Chemmac, which agreed with pH measured in the laboratory. The reason for this discrepancy is most likely changes in pressure, which affect the carbonate system.

The measurement sequences of Eh, pH, electrical conductivity, dissolved oxygen and water temperature are plotted versus time in Appendices 5 to 8.

The measurement data sequences 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 measurement sequences where the electrodes show stable values, marked with an arrow. The evaluated results from the measurements in the four investigated sections are given in Table 8-1.

8.2 Water analyses

8.2.1 Basic water analyses

The basic water analyses include Na, K, Ca, Mg, Fe, Li, Mn, S, Sr, P, SO_4^{2-}, Cl^-, Si, HCO_3^-, Br^-, F^-, I^-, HS^-, NH_4^+, NO_2^-, NO_3^-, TOC and DOC. 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 10, Table A10-1. Existing batch measurement values of pH and/or electrical conductivity are compared with the corresponding on-line Chemmac measurement values in Appendices 5 to 8.

Table 8-1. Evaluated results from the Chemmac measurements in KLX03.

Borehole section (m)	Electrical conductivity* (mS/m)	pH (borehole chemmac)**	pH (surface chemmac)**	Eh (borehole and surface chemmac)** (mV)	Dissolved oxygen*** (mg/L)
193.5–198.4	137 ± 4	8.1 ± 0.6 [1]	8.2 ± 0.2	–285 ± 19 [B]	0
408.0–415.3	494 ± 15	7.9 ± 0.6 [1]	7.9 ± 0.2	–271 ± 6 [Y]	0
735.5–748.0	1,173 ± 35	7.1 ± 0.6 [1]	7.5 ± 0.1	–210 ± 11 [B]	0–0.4
964.5–975.2	2,800 ± 84	8.3 ± 0.2	8.6 ± 0.2	–118 ± 35 [C]	0

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

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

*** Measuring interval 0–15 mg/L, resolution and measurement uncertainty ± 0.0001 mg/L.

[1] = The calculation is based on one glass electrode.

[B] = Only values from borehole Chemmac have been used in the calculation.

[Y] = Only values from surface Chemmac have been used in the calculation.

[C] = The calculation is based on the electrode (carbon) with the most negative potential.

The charge balance errors give an indication of the quality and uncertainty of the analyses of major constituents. The errors did exceed ± 5% in one case, no. 10075 from section 964.5–975.2 m, probably due to low concentrations of calcium and sodium. 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 Figures 8-1 and 8-2. The flushing water 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 sections 193.5–198.4 m and 964.5–975.2 m.

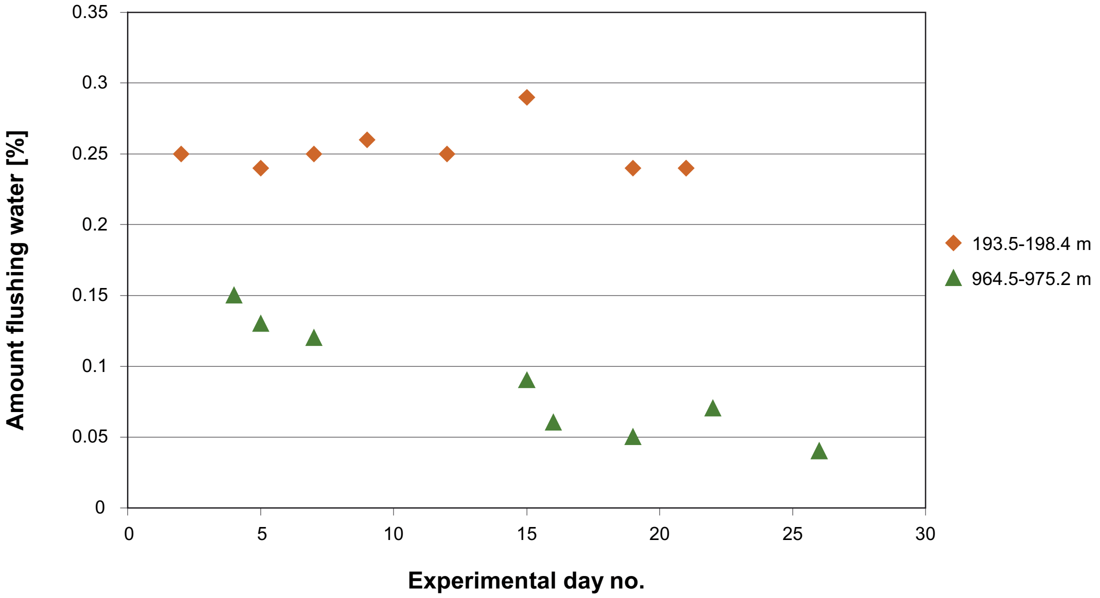


***Figure 8-1.** Flushing water content versus experimental day number, sections 193.5–198.4 m and 964.5–975.2 m.*

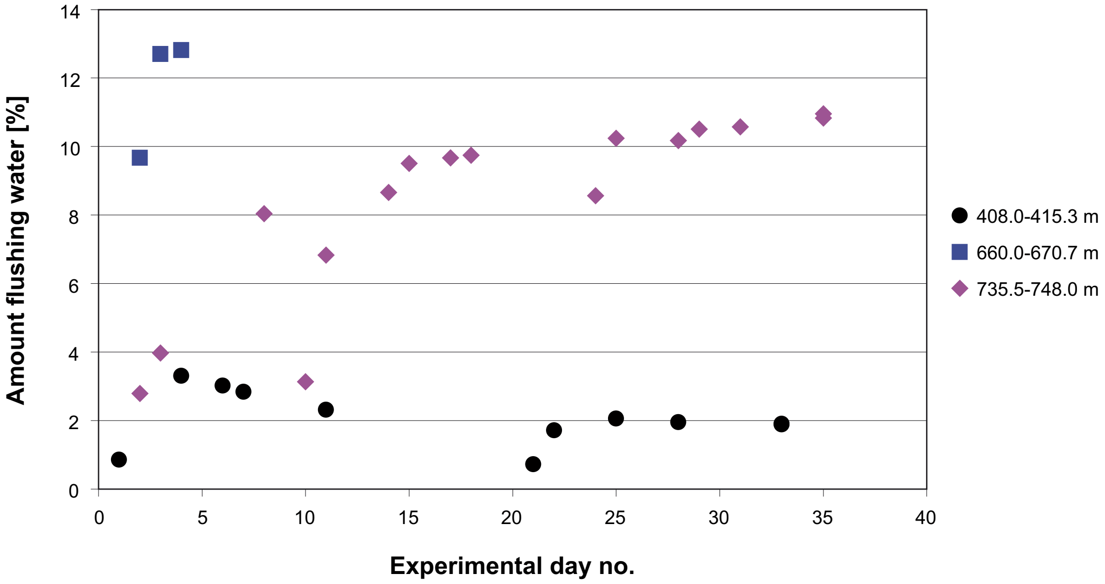


***Figure 8-2.** Flushing water content versus experimental day number, sections, 408.0–415.3, 660.0–670.7 and 735.5–748.0 m.*

However, in sections 408.0–415.3, 660.0–670.0 and 735.5–748.0 m, the flushing water content was 2, 13 and 11%, respectively, in the final water sample. The flushing water content in the samples is calculated using the average Uranine concentration in the added flushing water during core drilling.

The concentration levels of sodium, calcium and chloride are presented in Figures 8-3 to 8-7. The concentrations of all major constituents remained practically constant during the pumping and sampling periods except for in section 735.5–748.0 m, where an increasing concentration trend was observed.

The iron concentrations determined by ICP-AES (total Fe) and by spectrophotometry (Fe(+II) and Fe-tot) are compared in Figures 8-7 to 8-10 The total iron concentrations determined by ICP agree reasonably well with the results obtained by spectrophotometry. However, in a few cases, most obvious in section 735.5–748 m, the ICP results are somewhat lower. The ICP technique makes no distinction between different iron-containing species. Any colloidal iron present in a sample would give the opposite effect, as the spectrophotometric method excludes (or only partly includes) colloids, while the ICP technique makes no distinction between different iron-containing species.

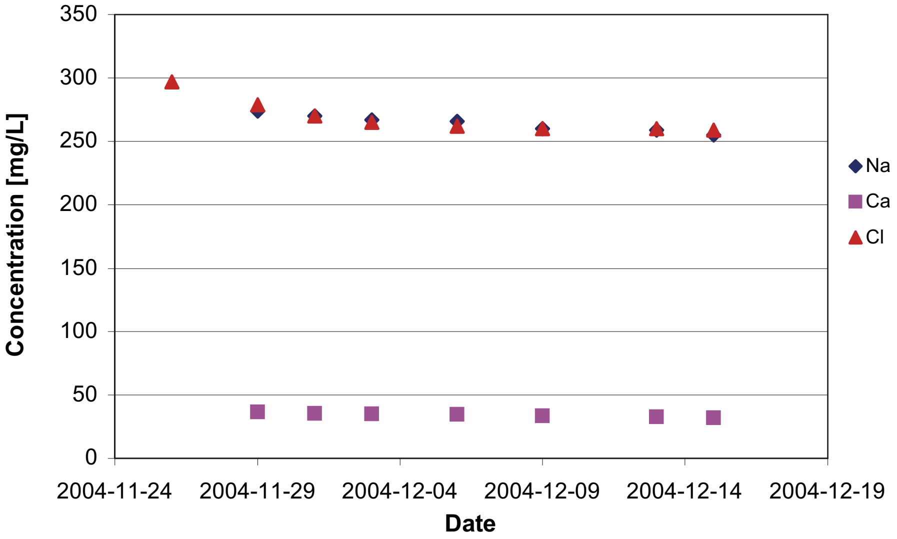


***Figure 8-3.** Sodium, calcium and chloride concentration trends from sample series at 193.5–198.4 m.*

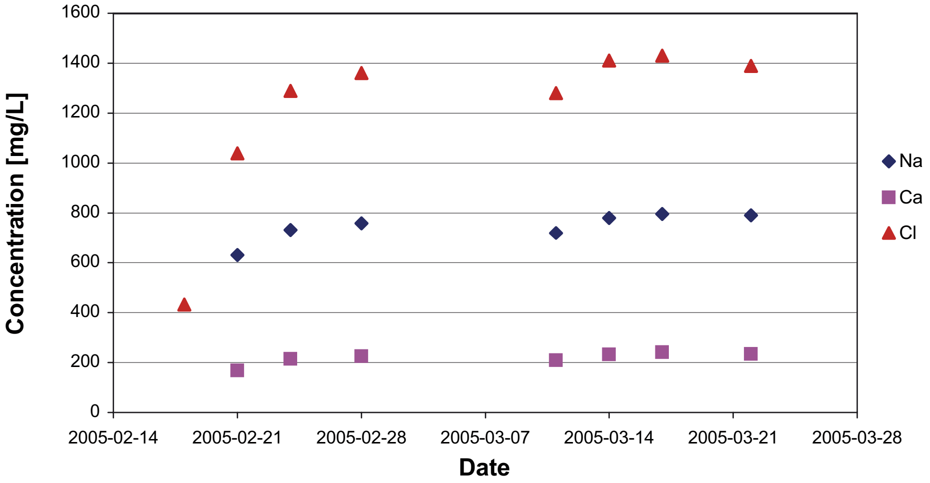


***Figure 8-4.** Sodium, calcium and chloride concentration trends from sample series at 408.0–415.3 m.*

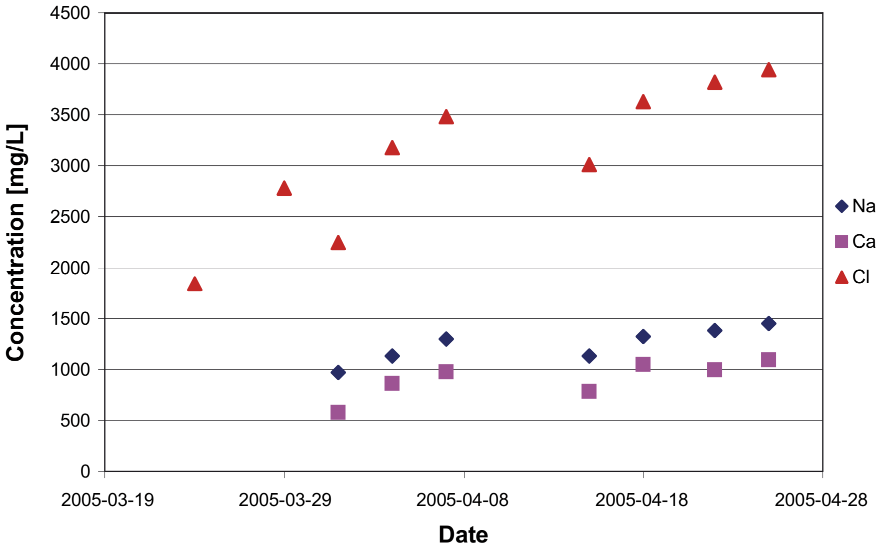


__Figure 8-5.__ Sodium, calcium and chloride concentration trends from sample series at 735.5–748.0 m.

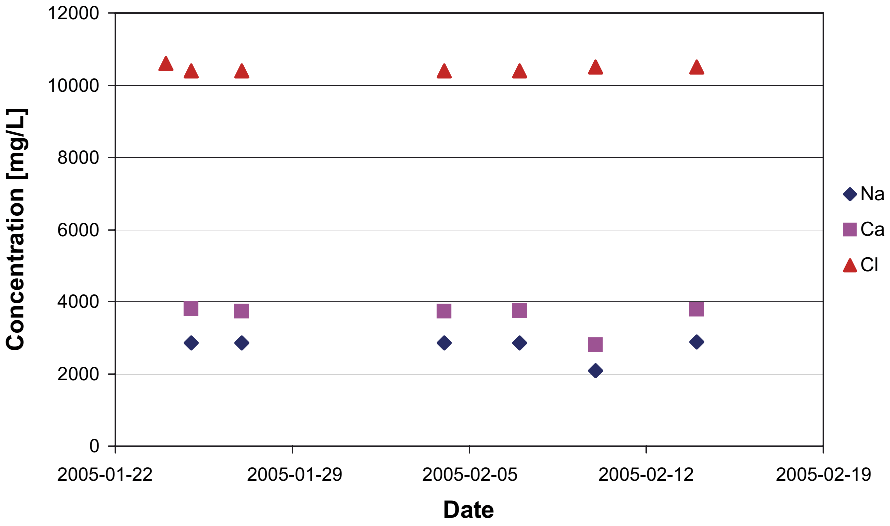


__Figure 8-6.__ Sodium, calcium and chloride concentration trends from sample series at 964.5–975.2 m.

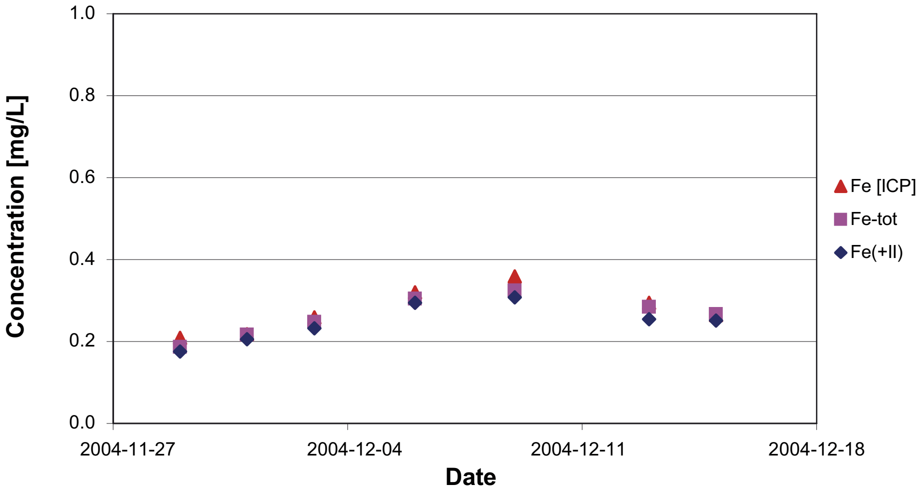


__Figure 8-7.__ Comparison of iron concentrations obtained by ICP-AES and spectrophotometry from borehole section 193.5–198.4 m.

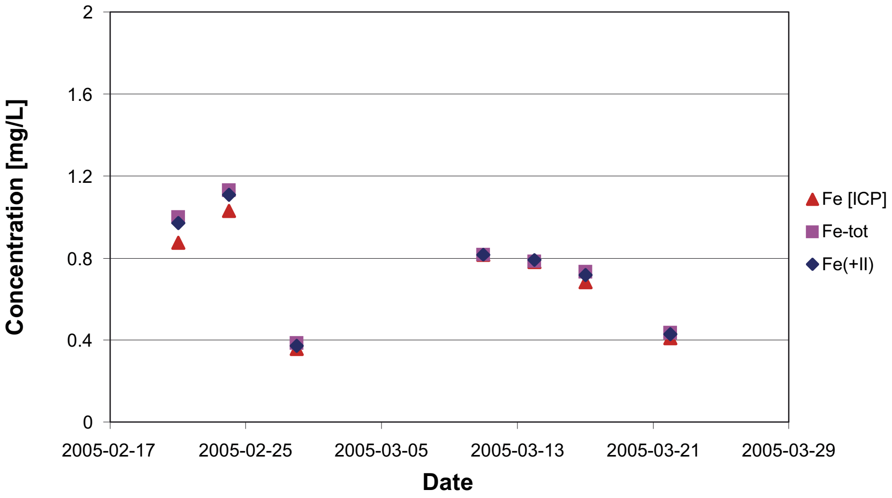


Figure 8-8. *Comparison of iron concentrations obtained by ICP-AES and spectrophotometry from borehole section 408.0–415.3 m.*

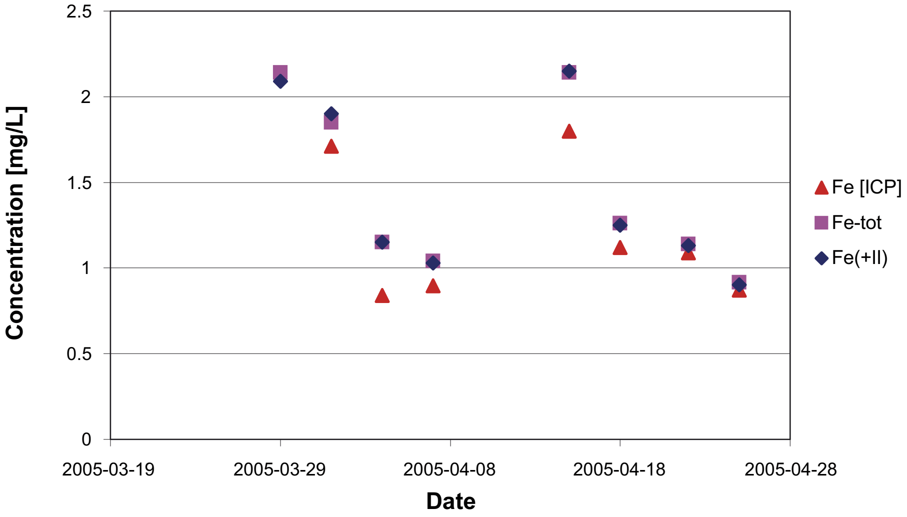


Figure 8-9. *Comparison of iron concentrations obtained by ICP-AES and spectrophotometry from borehole section 735.5–748.0 m.*

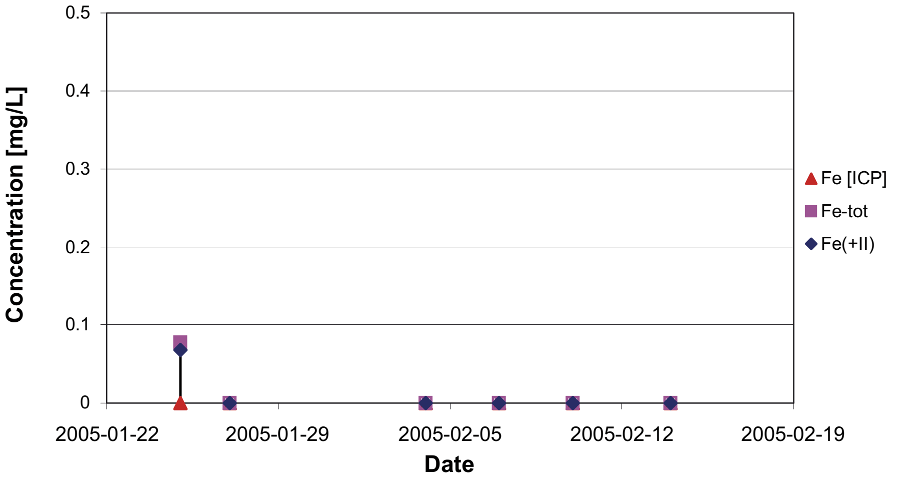


Figure 8-10. *Comparison of iron concentrations obtained by ICP-AES and spectrophotometry from borehole section 964.5–975.2 m.*

Sulphate analysed by ion chromatography (IC) is compared to sulphate determined as total sulphur by ICP-AES in Figures 8-11 to 8-14. The IC results are somewhat higher in section 193.5–198.4, 408.0–415.3 and 735.5–748.0 m while section 964.5–975.2 m shows the opposite. Experience has shown that ICP measurements may be more reliable since the variation between the samples in a time series often is smaller. The sulphate concentration remained constant during the investigation in sections 193.5–198.4 and 964.5–975.2 m while increasing trends are observed for sections 408.0–415.3 and 735.5–748.0 m.

The DOC results from the borehole sections are plotted versus experimental day number in Figure 8-15. DOC analyses in saline waters are, by experience, considered less reliable than in fresh waters.

The chloride concentrations are plotted versus the corresponding electrical conductivity values in Figure 8-16. The plot gives a rough check of the data. As shown, the data from the borehole sections agree well with the regression line obtained by earlier data from the Äspö Hard Rock Laboratory.

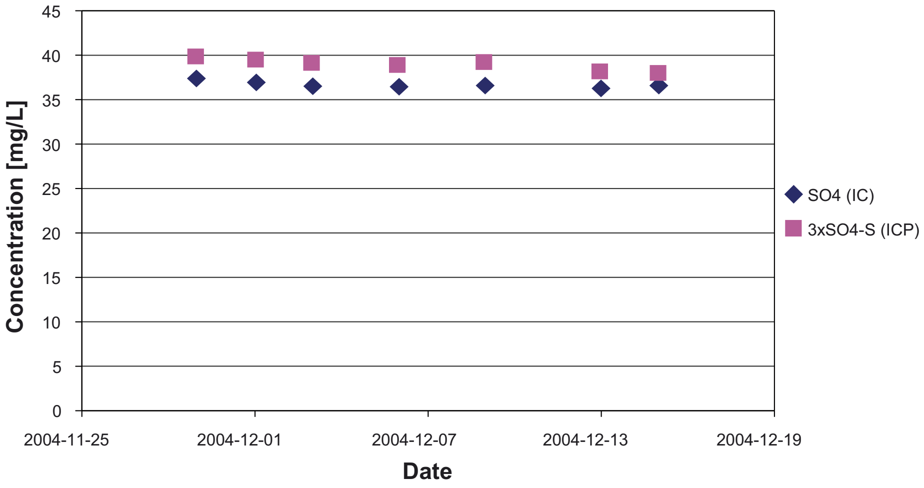


***Figure 8-11.** Sulphate (SO_4 by IC) to sulphate calculated from total sulphur ($3\times SO_4$-S by ICP) versus date. Samples in section 193.5–198.4 m.*

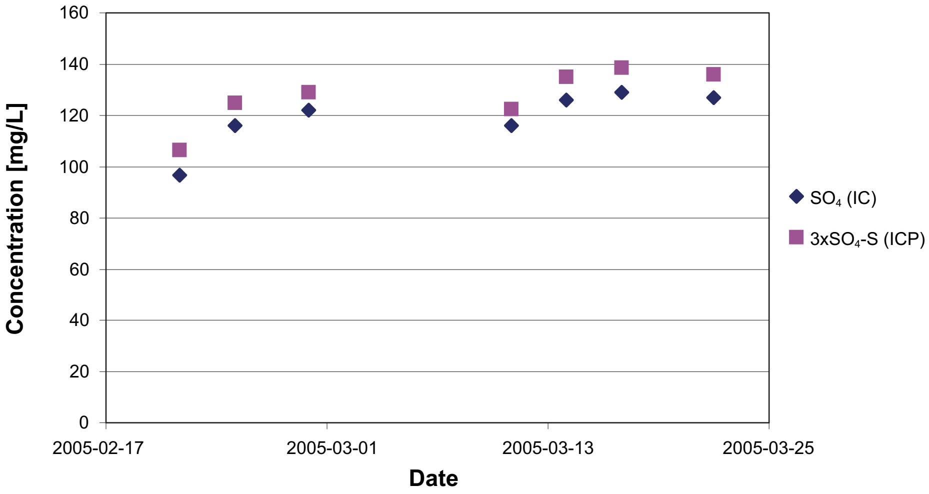


***Figure 8-12.** Sulphate (SO_4 by IC) to total total sulphate calculated from total sulphur ($3\times SO_4$-S by ICP) versus date. Samples collected collected in section 408.0–415.3 m.*

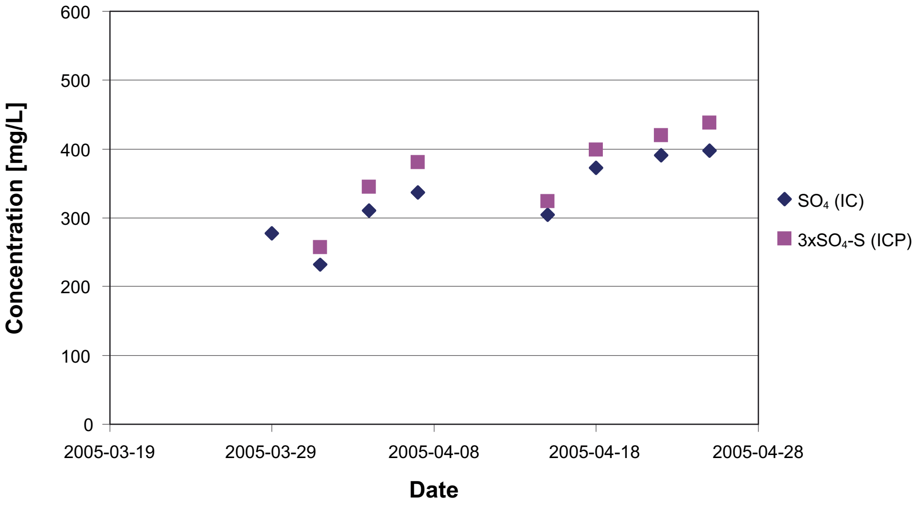


Figure 8-13. *Sulphate (SO_4 by IC) to total sulphate calculated from total sulphur (3×SO_4-S by ICP) versus date. Samples collected in section 735.5–748.0 m.*

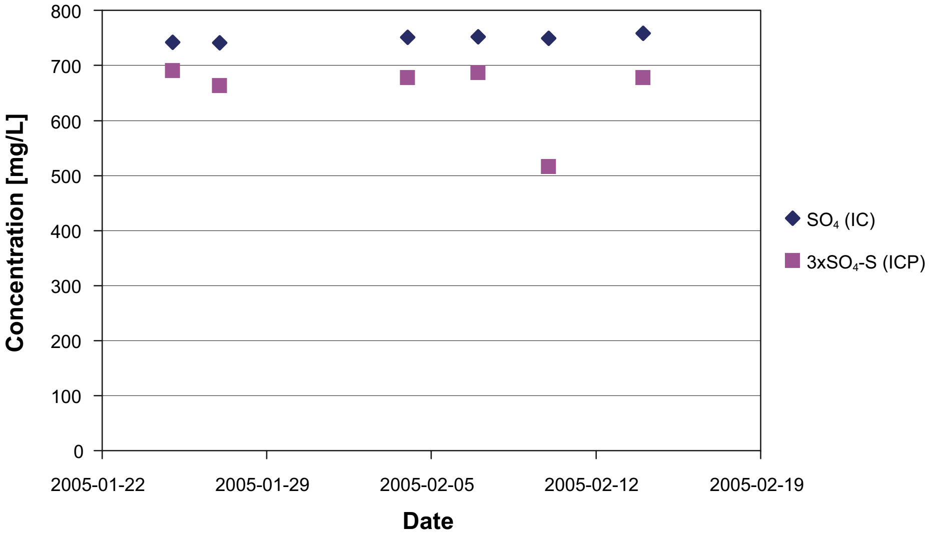


Figure 8-14. *Sulphate (SO_4 by IC) to total sulphate calculated from total sulphur (3×SO_4-S by ICP) versus date. Samples collected in section 964.5–975.2 m.*

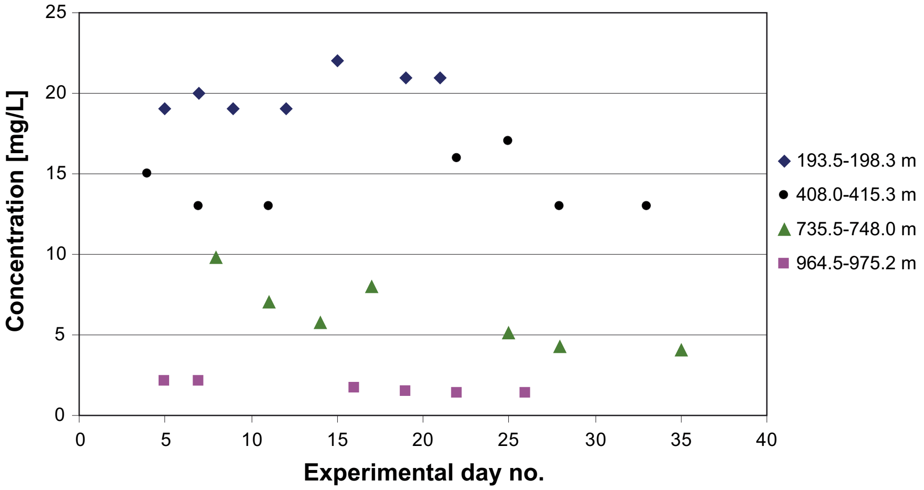


Figure 8-15. *DOC concentrations versus experimental day number.*

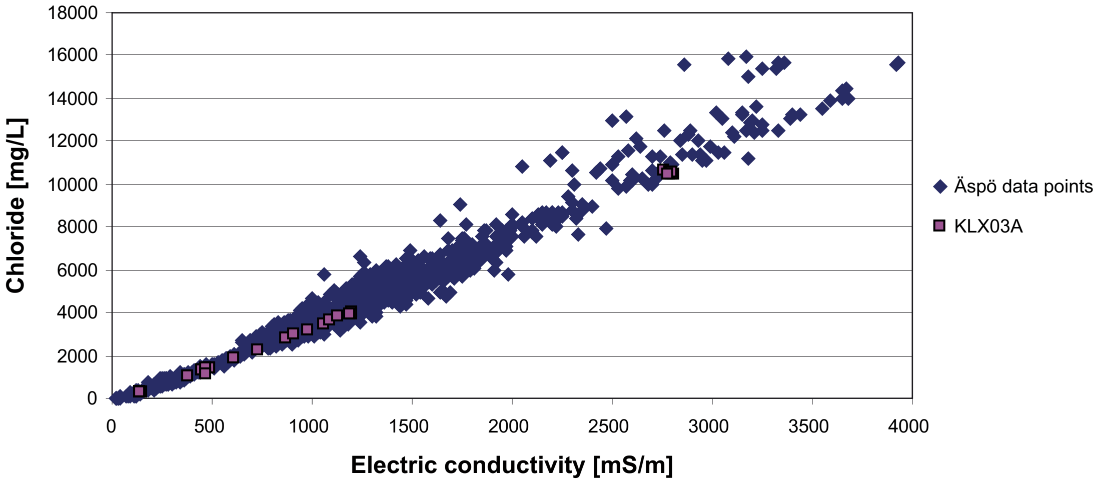


Figure 8-16. *Chloride concentration versus electrical conductivity. Data from earlier investigations at the Äspö Hard Rock Laboratory are used to show the linear relationship. The data from KLX03 do not deviate significantly from a thought regression line.*

8.2.2 Trace elements (rare earth metals and others)

The analyses of trace and rare earth metals include U, Th, As, Sc, Cd, Hg, V, Rb, Y, Zr, In, Cs, Ba, 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. The trace element data are compiled in Appendix 10, Table A10-3.

8.2.3 Stable and radioactive isotopes

The isotope determinations include the stable isotopes δD, $\delta^{18}O$, $^{10}B/^{11}B$, $\delta^{34}S$, $\delta^{13}C$ 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. Isotope data are compiled in Appendix 10, Table A10-2.5

The carbon isotopes ($\delta^{13}C$ and pmC) were determined both in inorganic carbon (hydrogen carbonate) and in organic constituents. The results are presented in Table 8-2 below. Enrichment of organic carbon was necessary in order to collect enough organic material.

A comparison between re-calculated uranium and thorium isotope determinations and ICP-analyses are given in Table 8-3. The isotopes uranium-238 and thorium-232 are converted to element concentrations using the expressions given in Appendix 9. Generally, results within the same order of magnitude indicate a satisfactory agreement.

Table 8-2. Inorganic and organic $\delta^{13}C$ and pmC.

Borehole section (m)	Inorg. $\delta^{13}C$ (dev PDB)	Org. $\delta^{13}C$ (dev PDB)	Inorg. pmC	Org. pmC
193.5–198.4	–17.0	–26.3	45.7	68.7
408.0–415.3	***	–27.1	***	65.2
735.5–748.0	**	*	**	*
964.5–975.2	**	–23.4	**	81.4

* Enrichment not performed due to high amount of remaining flushing water.

** No result, analytical procedure could not be performed due to low alkalinity.

*** No result due to problem with the postal service.

Table 8-3. Comparison of isotope determinations (^{238}U and ^{232}Th) and ICP-analyses of uranium and thorium.

Borehole section (m)	Sample no.	Date	U (µg/L)	U* (µg/L)	Th (µg/L)	Th** (µg/L)
193.5–198.4	7953	2004-12-15	0.631	< 4.0	0.104	< 12.7
408.0–415.3	10091	2005-03-22	0.421	< 4.0	0.0402	< 12.7
735.5–748.0	10242	2005-04-25	0.127	< 4.0	< 0.4	< 12.7
964.5–975.2	10076	2005-02-14	< 0.01	< 4.0	< 0.2	< 12.7

* Recalculated from ^{238}U (mBq/L).

** Recalculated from ^{232}Th (mBq/L).

8.3 Dissolved gas

Sampling for gas was performed in sections 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m. The analyses of dissolved gases include argon (Ar), helium (He), nitrogen (N_2), carbon dioxide (CO_2), carbon monoxide (CO) methane (CH_4), oxygen (O_2), hydrogen (H_2), ethane (C_2H_6), ethene (C_2H_4), ethyne (C_2H_2), propane (C_3H_8) and propene (C_3H_6). Carbon monoxide was not analysed in samples from sections 408.0–415.3 m and 964.5–975.2 m. The gas data are compiled in Appendix 10, Table A10-5.

Total gas content in the groundwater as well as the detected oxygen content is given in Table 8-4. The oxygen concentration was especially high in gas samples from section 193.5–198.4 m. The oxygen content indicates air leakage into the purging system at the consulted laboratory. The air leakage which affects the analysis results may be corrected, assuming that the oxygen content is zero, by removing the air effect (nitrogen, oxygen and argon).

The gas composition of the four different borehole sections is compared in Figures 8-17 and 8-18. The results from the carbon monoxide analysis were below the reporting limit in sections 193.5–198.4 m (< 3.1 µL/L) and 735.5–748.0 m (< 3.3 µL/L).

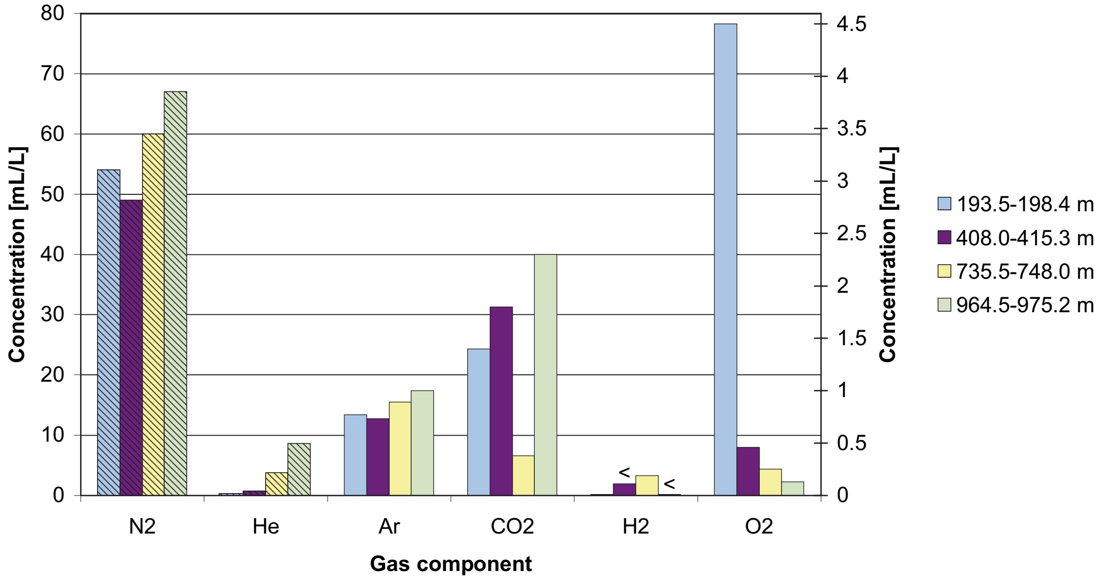


Figure 8-17. *Gas components of high concentrations (N_2, He, Ar, CO_2, H_2 and O_2) in samples collected in KLX03 using the in situ sampling equipment. Striped and non-striped bars refer to the scales on left and right axis, respectively.*

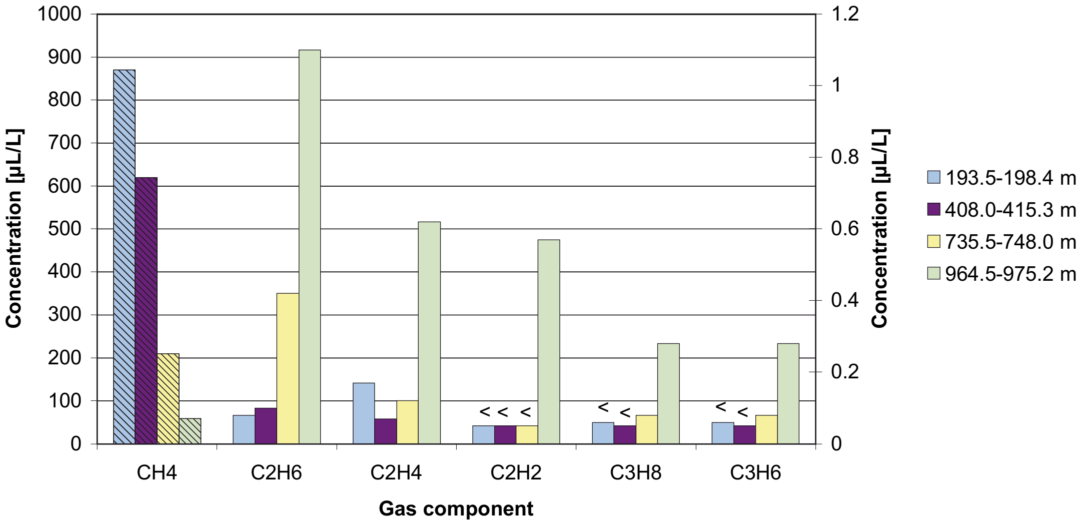


***Figure 8-18**. Gas components of low concentrations (CH_4, C_2H_6, C_2H_4, C_2H_2, C_3H_8 and C_3H_6) in samples collected in KLX03A using the in situ sampling equipment. Striped and non-striped bars refer to the scales on left and right axis, respectively.*

Table 8-4. Total content of dissolved gas.

	Section 193.5–198.4 m	Section 408.0–415.3 m	Section 735.5–748.0 m	Section 964.5–975.2 m
Total gas content (mL/L)	62	53	66	76
Oxygen content (mL/L)	4.5	0.46	0.25	0.13

8.4 Inorganic colloids

The presence of inorganic colloids was investigated by two different methods. One method was colloid filtration through a series of connected filters of different pore sizes. A second method was fractionation/ultra filtration using cylindrical membrane filters with a cut-off of 1,000 D and 5,000 D, respectively. The results from the two methods are difficult to compare quantitatively but a qualitative agreement is identified.

8.4.1 Inorganic colloids – colloid filtration

The results from the colloid filtration performed in sections 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m are presented in Figures 8-19 to 8-22, Figures 8-23 to 8-26, Figures 8-27 to 8-30 and Figures 8-31 to 8-34, respectively.

The bars in the diagrams represent amounts (µg) of aluminium, iron, silicon and manganese 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 in 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 taken on-line at the surface just before opening the PVB-containers for sampling.

Results of colloid filtering experiment, using water sample from section 193.5–198.4 m

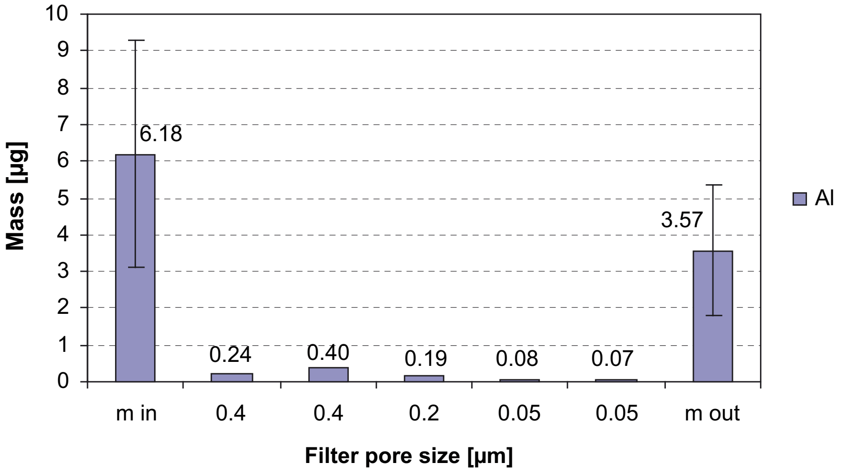


Figure 8-19. *Amount of aluminium entering the filter system (m in), in the filters and in the collecting container (m out).*

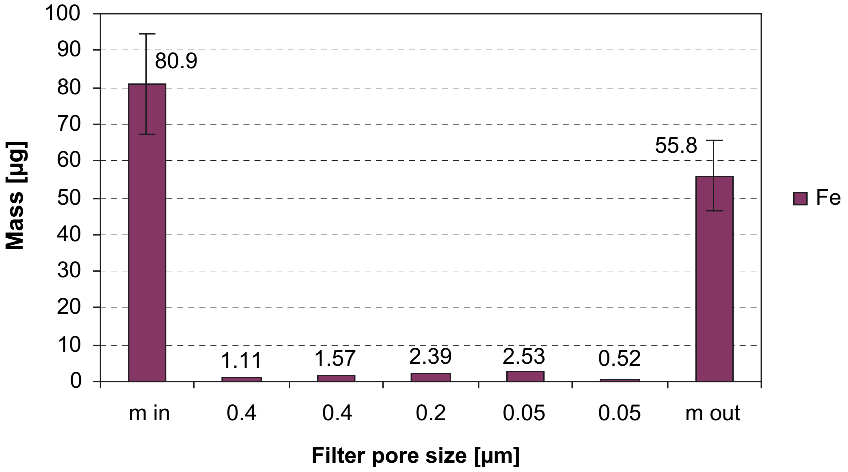


Figure 8-20. *Amount of iron entering the filter system (m in), in the filters and in the collecting container (m out).*

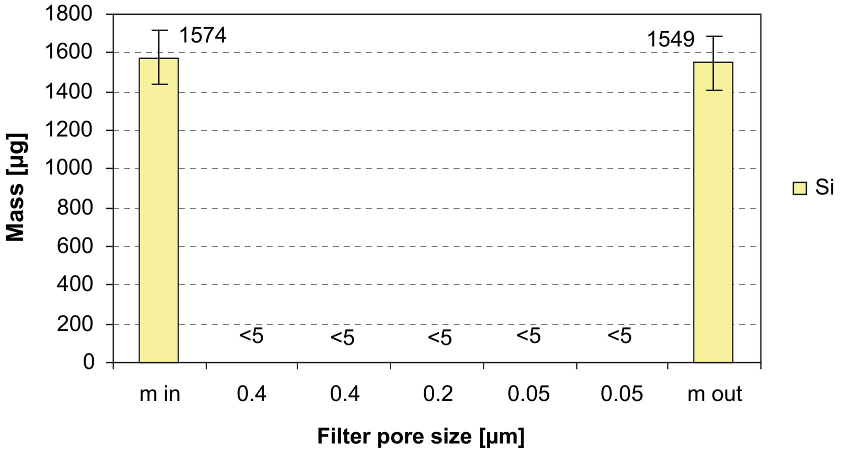


Figure 8-21. *Amount of silicon entering the filter system (m in), in the filters and in the collecting container (m out).*

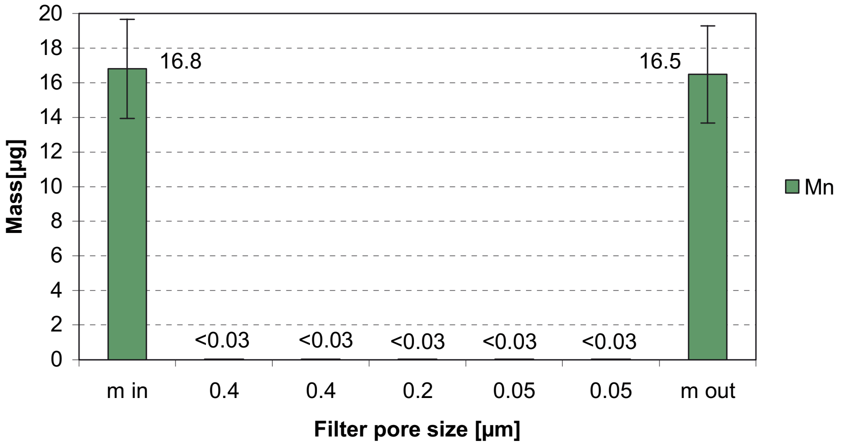


Figure 8-22. *Amount of manganese entering the filter system (m in), in the filters and in the collecting container (m out).*

Results of colloid filtering experiment, using water sample from section 408.0–415.3 m

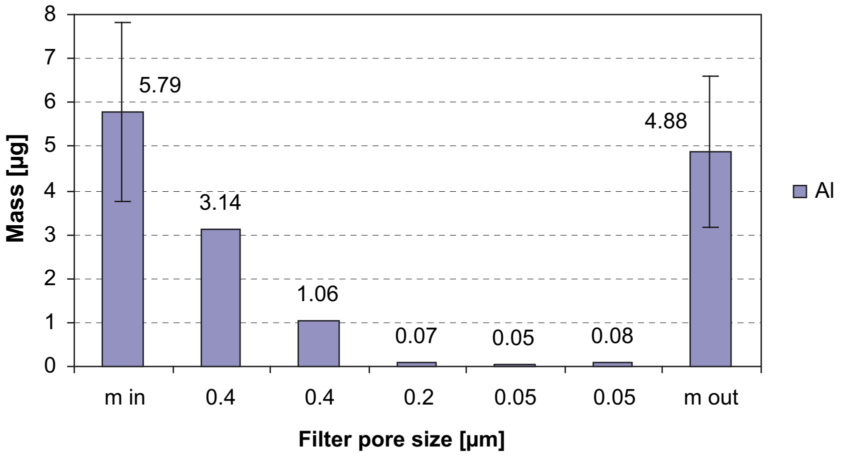


Figure 8-23. *Amount of aluminium entering the filter system (m in), in the filters and in the collecting container (m out).*

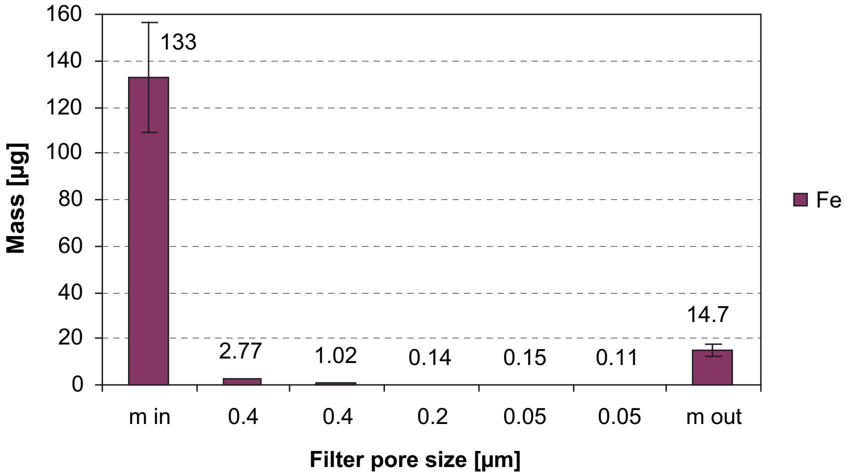


Figure 8-24. *Amount of iron entering the filter system (m in), in the filters and in the collecting container (m out).*

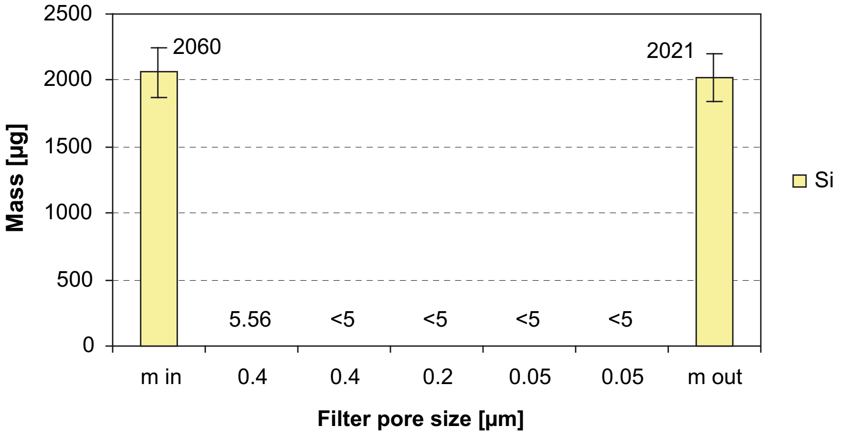


Figure 8-25. *Amount of silicon entering the filter system (m in), in the filters and in the collecting container (m out).*

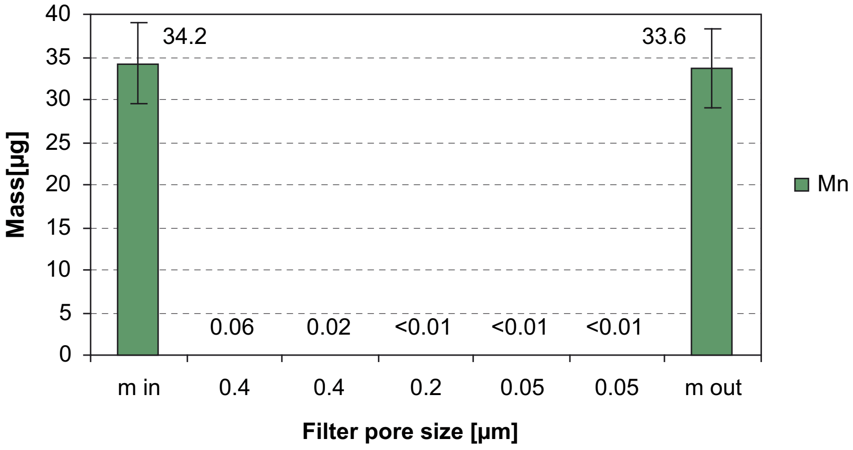


Figure 8-26. *Amount of manganese entering the filter system (m in), in the filters and in the collecting container (m out).*

Results of colloid filtering experiment, using water sample from section 735.5–748.0 m

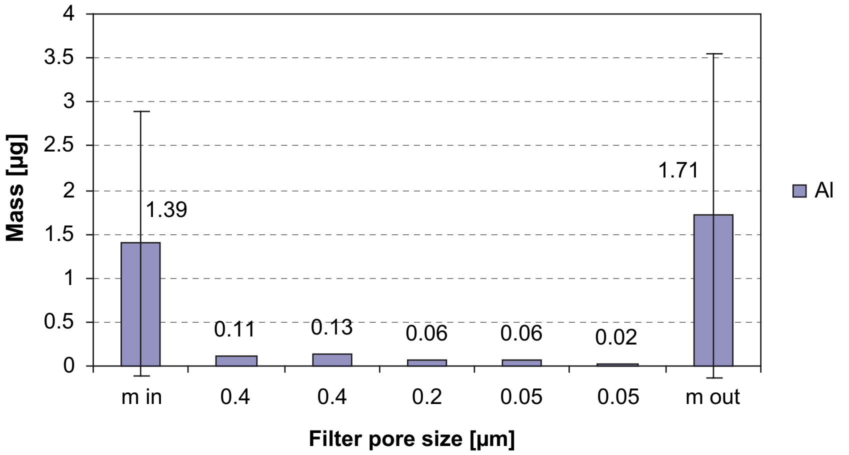


Figure 8-27. *Amount of aluminium entering the filter system (m in), in the filters and in the collecting container (m out).*

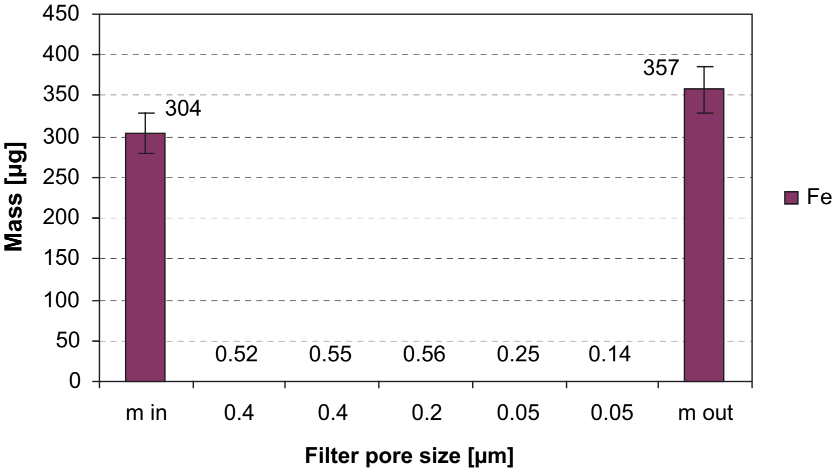


Figure 8-28. *Amount of iron entering the filter system (m in), in the filters and in the collecting container (m out).*

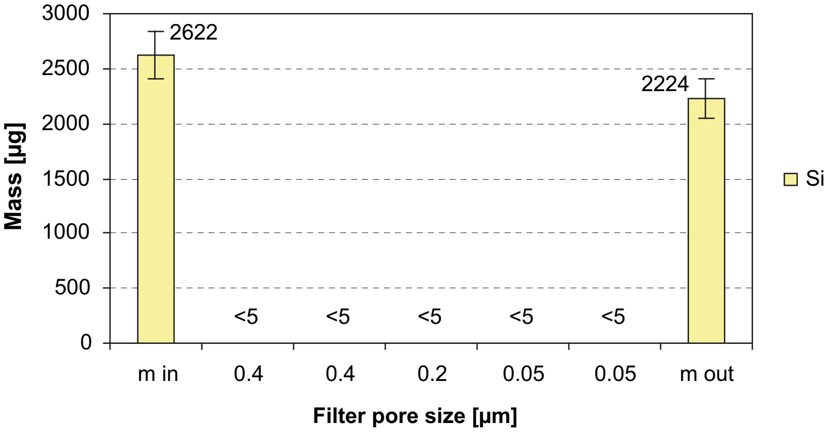


Figure 8-29. *Amount of silicon entering the filter system (m in), in the filters and in the collecting container (m out).*

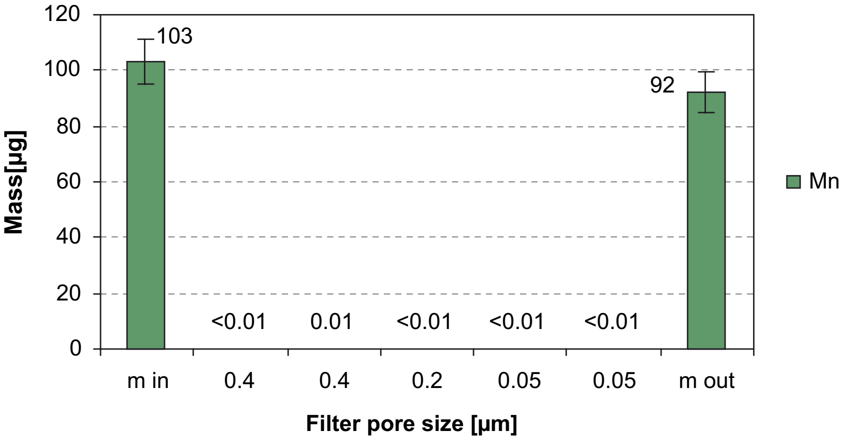


Figure 8-30. *Amount of manganese entering the filter system (m in), in the filters and in the collecting container (m out).*

Results of colloid filtering experiment, using water sample from section 964.5–975.2 m

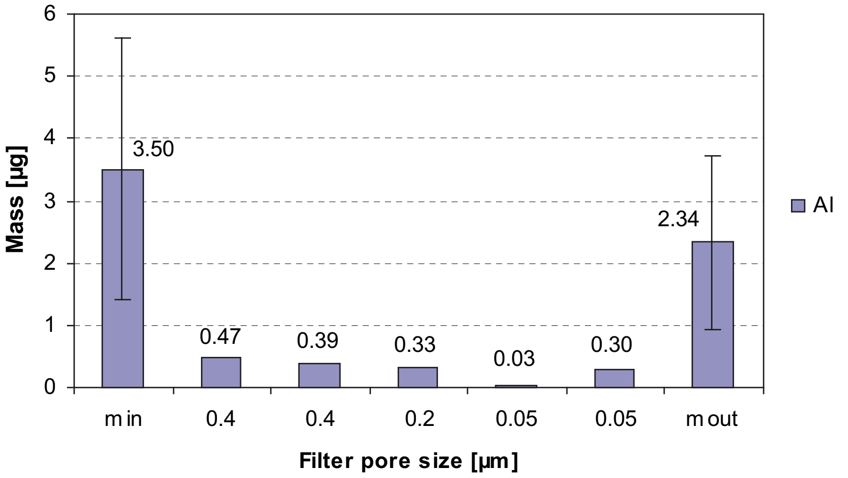


Figure 8-31. *Amount of aluminium entering the filter system (m in), in the filters and in the collecting container (m out).*

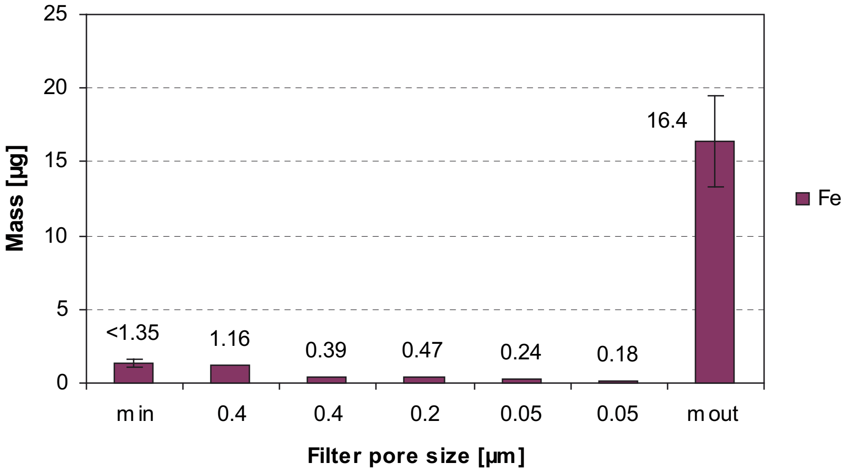


Figure 8-32. *Amount of iron entering the filter system (m in), in the filters and in the collecting container (m out).*

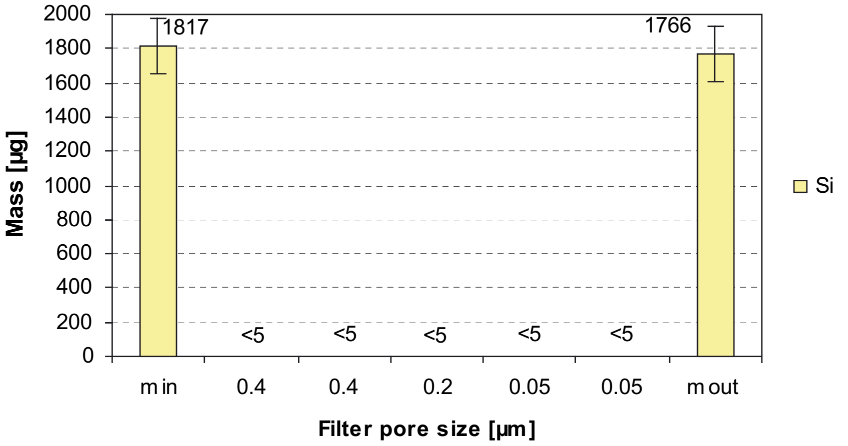


Figure 8-33. *Amount of silicon entering the filter system (m in), in the filters and in the collecting container (m out).*

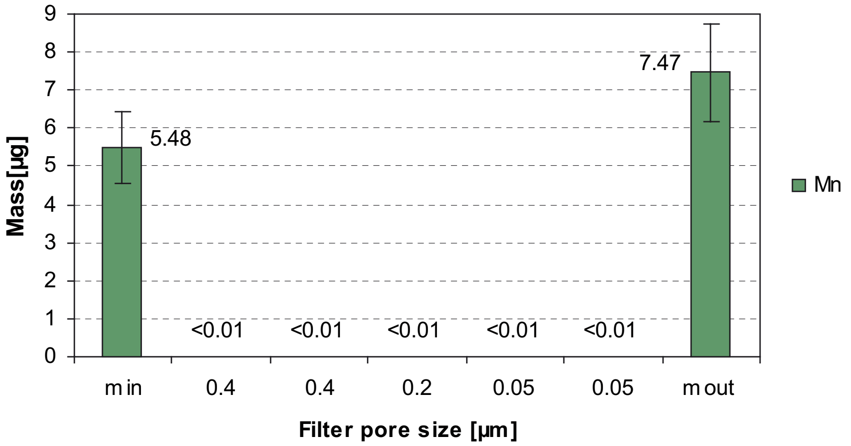


Figure 8-34. *Amount of manganese entering the filter system (m in), in the filters and in the collecting container (m out).*

The concentrations in blank samples (rinsing water), PVB-containers, collecting container and pumped groundwater are given in Table 8-5. The remaining water in the PVB containers after filtration was possibly contaminated by aluminium and iron. The evaluation is complicated for aluminium and iron since contamination and/or precipitation have to be considered.

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

The following may be concluded from the colloid filtration results:

- Aluminium and iron are somewhat difficult to evaluate since the output amount plus the amount incorporated on filters does not balance the input amount. As can be concluded from Table 8-5, the reasons for this are contamination and/or precipitation in the PVB-containers.
- Aluminium and iron are detected in significant amounts on the filters. Addition of these element amounts (0.4 µm pore size excluded) gives colloid concentrations of 21.2 µg/L, 2.0 µg/L, 3.3 µg/L and 4.6 µg/L for sections 193.5–198.4, 408.0–415.3, 735.5–748.0 and 964.5–975.2 m, respectively. The corresponding calculation using the amounts of real colloid species will give a somewhat higher value (example of colloid species $Fe(OH)_2$). It is probable that real background concentration of colloids is lower, since precipitated iron as well as contamination by iron and aluminium contributes.
- Silica and manganese are not above detection limit on the filters (0.4 µm pore size excluded).

Furthermore, the results show that Calcite did not precipitate to any significant extent during the colloid filtrations for section 193.5–198.4, 408.0–415.3 and 735.5–748.0 m.

8.4.2 Inorganic colloids – fractionation

Besides the DOC analyses, the samples from fractionation experiments were also analysed by ICP-AES. 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 and Zn. Only Fe (iron), Si (silicon), Ca (calcium), S (sulphur), Al (aluminium) and Mn (manganese) were considered important as colloid species. Fractionation was excluded in section 735.5–748.0 m due to a high content of flushing water.

Table 8-5. Concentrations in blank water, remaining water in PVB container, collected output water from filter system and pumped water that has not passed the filter system.

Section m	Sample origin	Al µg/L	Ca mg/L	Fe mg/L	Mn µg/L	Si mg/L
193.5–198.4	Blank, deionised water	4.53	< 0.1	< 0.0004	0.0642	0.102
	Blank, leakage test	3.2	0.3	0.072	18.3	0.276
	Pumped water (alt. input conc)	22.7	33.5	0.297	61.7	5.78
	Rest volume PVB (input conc)	220 924	34.1 35.3	1.40 4.61	73.6 98.4	6.39 8.30
	Collecting container	13.1	33.3	0.205	60.5	5.69
408.0–415.3	Blank, deionised water	0.703	< 0.1	0.0007	< 0.03	0.0922
	Blank, leakage test	2.61	< 0.1	0.0083	5.83	0.0305
	Pumped water (alt. input conc)	19.1	219.0	0.438	113	6.8
	Rest volume PVB (input conc)	30,200 28,800	218 217	38.7 36.5	772 732	70.8 64.4
	Collecting container	16.1	200	0.0485	111	6.67
735.5–748.0	Blank, deionised water	0.829	< 0.1	0.001	< 0.03	0.0924
	Blank, leakage test	4.47	< 1	0.0118	2.33	< 0.3
	Pumped water (alt. input conc)	4.16	1,120	0.911	308	7.84
	Rest volume PVB (input conc)	949 1,290	1,060 1,030	7.65 4.6	451 377	8.74 8.52
	Collecting container	5.11	951	1.07	276	6.65
964.5–975.2	Blank, deionised water	0.741	< 0.1	0.0008	< 0.03	0.0912
	Blank, leakage test	1.65	< 0.1	0.002	0.124	0.18
	Pumped water (alt. input conc)	10.4	3,810	< 0.004	16.3	5.40
	Rest volume PVB (input conc)	3,440 2,580	3,840 3,700	8.51 7.2	149 114	13.7 11.6
	Collecting container	6.94	3,680	0.0486	22.2	5.25

Blank, leakage test = remaining water in the PVB container after filtration of blank sample/de-ionised water. Pumped water = sample collected at the surface and not in situ in the borehole section.

Rest volume PVB = remaining water in the PVB container after filtration of sample. Collecting container = water that has passed the filter system.

The results presented in Tables 8-6 to 8-8 were calculated using mass balance equations (SKB MD 431.043). Silicon and aluminium exist as species (associated or non-associated with humic and fulvic acids) with a molecular weight less than 1,000 D (g/mol). Such species are too small to be referred to as colloids. The same is true for calcium, sulphur and manganese, except for section 193.5–198.4 m where fractions of calcium, sulphur and manganese have molecular weights over 1,000 D and 5,000 D, respectively. There is a possibility that the fractions of iron with molecular weight > 1,000 D but < 5,000 D and > 5,000 D originates from the filtering process itself (due to oxygen in the filtering system; pump, filter, hose etc). The total iron concentration in section 964.5–975.2 m was below the detection limit.

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 iron, silicon, aluminium and manganese were insignificant (within the error of the analyses). Calcite was not precipitated to any significant extent in any of the samples during the filtrations.

Table 8-6. Inorganic fractions (1,000 D and 5,000 D filters) in section 193.5–198.4 m.

Fraction	Fe (mg/L)	Si (mg/L)	Ca (mg/L)	S (mg/L)	Al (µg/L)	Mn (µg/L)
< 1,000 D	0.004 ± 0.001	5.7 ± 0.8	29.6 ± 3.6	10.8 ± 1.4	12.5 ± 8.8	57.0 ± 5.7
< 5,000 D	0.007 ± 0.001	5.6 ± 0.8	29.9 ± 3.6	11.1 ± 1.4	8.8 ± 6.1	54.0 ± 9.2
> 1,000 D but < 5,000 D	0.11 ± 0.01	–	–	–	–	–
> 5,000 D	0.22 ± 0.02	–	1.5 ± 1.1	0.9 ± 0.5	–	5.7 ± 3.4
Adsorption 1,000 D	–	–	–	–	–	–
Adsorption 5,000 D	0.05 ± 0.03	–	–	–	–	–

– = Not found.

Table 8-7. Inorganic fractions (1,000 D and 5,000 D filters) in section 408.0–415.3 m.

Fraction	Fe (mg/L)	Si (mg/L)	Ca (mg/L)	S (mg/L)	Al (µg/L)	Mn (µg/L)
< 1,000 D	0.001 ± 0.001	6.3 ± 0.6	216 ± 22	41.5 ± 5.4	10.5 ± 2.1	115 ± 12
< 5,000 D	0.009 ± 0.002	6.3 ± 0.6	219 ± 22	42.4 ± 5.5	7.4 ± 1.1	114 ± 11
> 1,000 D but < 5,000 D	–	–	–	–	–	–
> 5,000 D	0.23 ± 0.05	–	–	–	–	–
Adsorption 1,000 D	0.52 ± 0.35	–	–	–	–	–
Adsorption 5,000 D	0.32 ± 0.12	–	–	–	–	–

– = Not found.

Table 8-8. Inorganic fractions (1,000 D and 5,000 D filters) in section 964.5–975.2 m.

Fraction	Fe (mg/L)	Si (mg/L)	Ca (mg/L)	S (mg/L)	Al (µg/L)	Mn (µg/L)
< 1,000 D	< 0.004	5.0 ± 0.5	3,500 ± 420	222 ± 29	7.4 ± 5.2	18.1 ± 3.1
< 5,000 D	< 0.004	5.1 ± 0.5	3,540 ± 425	231 ± 30	6.6 ± 4.6	19.3 ± 3.3
> 1,000 D but < 5,000 D	–	–	–	–	–	–
> 5,000 D	–	–	–	–	–	–
Adsorption 1,000 D	–	–	–	–	–	–
Adsorption 5,000 D	–	–	–	–	–	–

– = Not found.

8.5 Humic and fulvic acids

The results from fractionation of organic acids in sections 193.5–198.4, 408.0–415.3 and 964.5–975.2 m are summarised in Table 8-9. As shown, the water in sections 193.5–198.4 m and 408.0–415.3 m contain a fraction of organic acids with a molecular weight above 5,000 D while in the deepest section, 964.5–975.2 m, the organic acids have a molecular weight of less than 1,000 D. The organic acids in this fraction consist of fulvic acids and possibly other low molecular weight organic acids such as citric acid and oxalic acid. The results from the 1,000 D and 5,000 D filters were consistent for all sections.

Table 8-9. Summary of fractionation results in KLX03.

Fraction	Section 193.5–198.4 m DOC (mg/L)	Section 408.0–415.3 m DOC (mg/L)	Section 964.5–975.2 m DOC (mg/L)
< 1,000 D	6.2 ± 0.7	5.9 ± 0.8	1.4 ± 0.2
> 1,000 D but < 5,000 D	1.2 ± 0.1	1.4 ± 0.1	–
> 5,000 D	11.5 ± 1.5	4.5 ± 0.8	–

– = Not found.

9 Summary

The *Complete chemical characterisation* in KLX03 was, on the whole, performed successfully.

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 condition was met in sections 193.5–198.4 m and 964.5–975.2 m but not in sections 408.0–415.3 m (3%) and 735.5–748.0 m (11%).
- The salinity was stable during the pumping and sampling periods, except for in section 735.5–748.0 m, were a slightly increasing concentration trend was recognised. A stable salinity indicates that there was no contribution of water from more distant fracture systems with a different water composition.
- The redox potential measurements made using the downhole Chemmac in sections 193.5–198.4, 408.0–415.3 and 735.5–748.0 m appear to be of good quality. The three electrodes (gold, glassy carbon and platinum) reached stable and consistent values (–285, –271 and –210 mV, respectively). Positive redox potentials were indicated by the electrodes in surface Chemmac except for section 408.0–415.3 m, where the potentials given by the surface electrodes corresponded to the potentials of the borehole electrodes. Possible reasons for the discrepancy between borehole and surface electrode potentials may be air intrusion or gas bubbles on electrode surfaces. The redox measurements in section 964.5–975.2 m did not show consistent values during the measurement period. This is probably due to the very low iron concentration in this section and thereby the lack of a dominating redox pair.
- The pH electrodes in the borehole Chemmac generally give lower values than those in surface Chemmac and pH measured in the laboratory.
- The results from colloid filtering and fractionation using ultra-filtration indicate that the content of silicon and manganese colloids in the groundwater is low or non-existent. The evaluation is more complicated for aluminium and iron since in both methods possible contamination and/or precipitation have to be considered.
- The organic constituents in the groundwater are present as fulvic acids and possibly other low molecular weight organic acids such as citric acid and oxalic acid in section 964.5–975.2 m. In sections 193.5–198.4 and 408.0–415.3 m, there is also a significant fraction of organic acids (humic acids) larger than 5,000 D.
- Comparison of results from different laboratories and/or methods did show agreement in most cases. The charge balance error exceeds the limit, ± 5%, in one water sample, SKB sample number 10075, section 964.5–975.2 m. Generally SKB sample number 10075 have lower values than SKB sample number 10074 and 10076. No results from water samples were considered unconfident, based on general trends. The investigation at section at 660.0–670.7 m is not relevant, due to limited amounts of data to compare.

10 References

/1/ **SKB, 2001.** Site investigations. Investigation methods and general execution programme. SKB TR-01-29, Svensk Kärnbränslehantering AB.

/2/ **Pedersen K, 2005.** Oskarshamn site investigation. Numbers and metabolic diversity of microorganisms in borehole KLX03. Results from sections 193.5–198.4, 408.0–415.3, 735.5–748.0, 964.5–975.2 m. SKB P-05-182, Svensk Kärnbränslehantering AB.

/3/ **Berg C, Wacker P, 2004.** Oskarshamn site investigation. Hydrochemical logging in KLX03. SKB P-04-299**,** Svensk Kärnbränslehantering AB.

/4/ **Gustafsson J, Gustafsson C, 2004.** Oskarshamn site investigation. RAMAC and BIPS logging in boreholes KLX03, HAV11 to HAV13 and HLX21 to HLX25. SKB P-04-275, Svensk Kärnbränslehantering AB.

/5/ **Nielsen U T, Horn F, 2005.** Oskarshamn site investigation. Geophysical borehole logging in borehole KLX03, HLX21, HLX22, HLX23, HLX24 and HLX25. SKB P-04-280, Svensk Kärnbränslehantering AB.

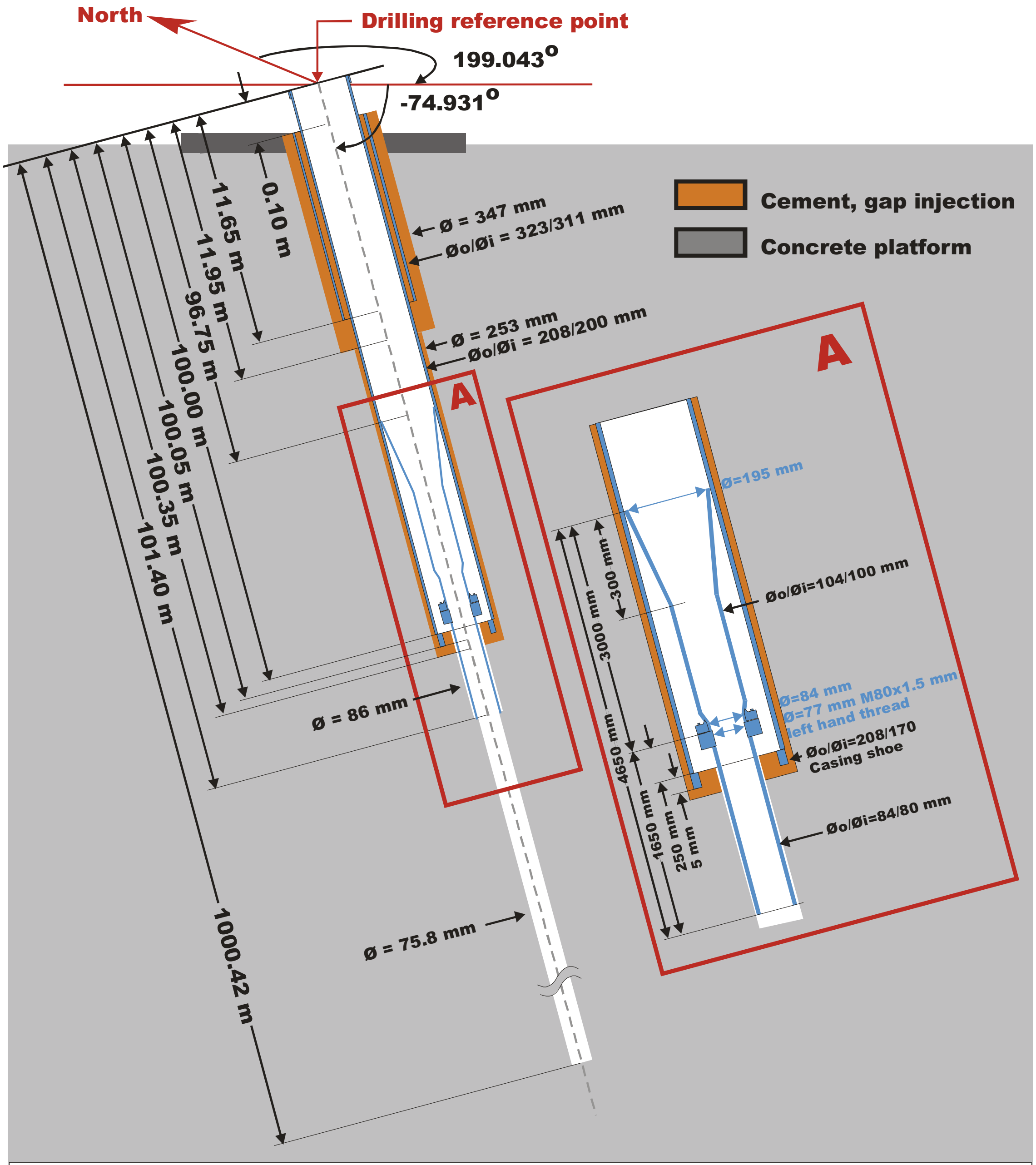
/6/ **Rouhiainen P, Pöllänen J, Sokolnicki M, 2005.** Oskarshamn site investigation. Difference flow logging of borehole KLX03. Subarea Laxemar. SKB P-05-67, Svensk Kärnbränslehantering AB.

Appendix 1

Design of cored borehole KLX03

Technical data

Borehole KLX03



Drilling reference point

Northing: 6366112.59 (m), RT90 2,5 gon V 0:-15
Easting: 1547718.93 (m), RT90 2,5 gon V 0:-15
Elevation: 18.49 (m), RHB 70

Drilling period

Drilling start date: 2004-05-03
Drilling stop date: 2004-09-07

Appendix 2

Results of difference flow logging in KLX03

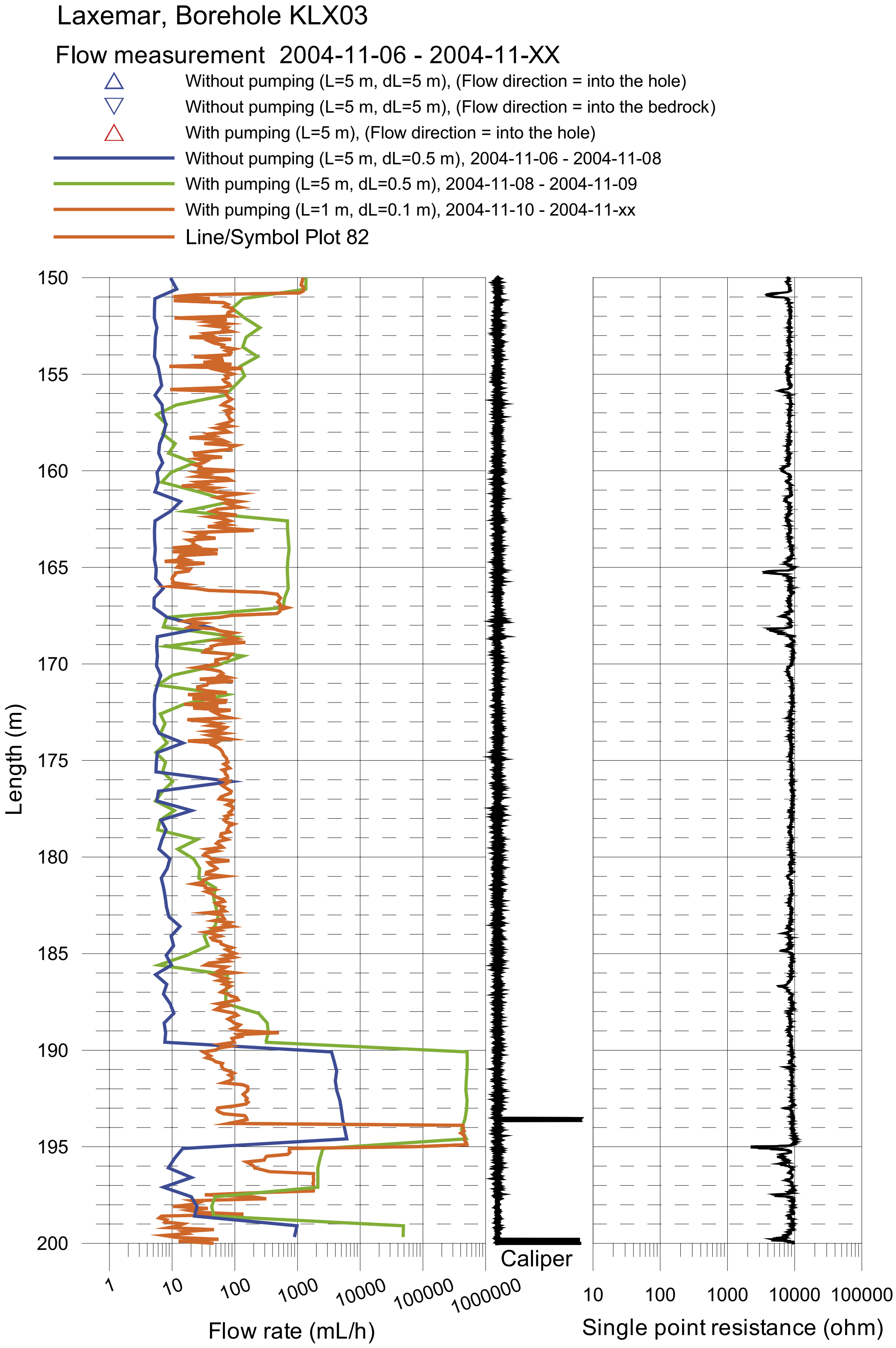


Figure A2-1. Borehole KLX03A: Differential flow measurements from 150–200 m including the water bearing fracture zone at approximately 195 m /6/.

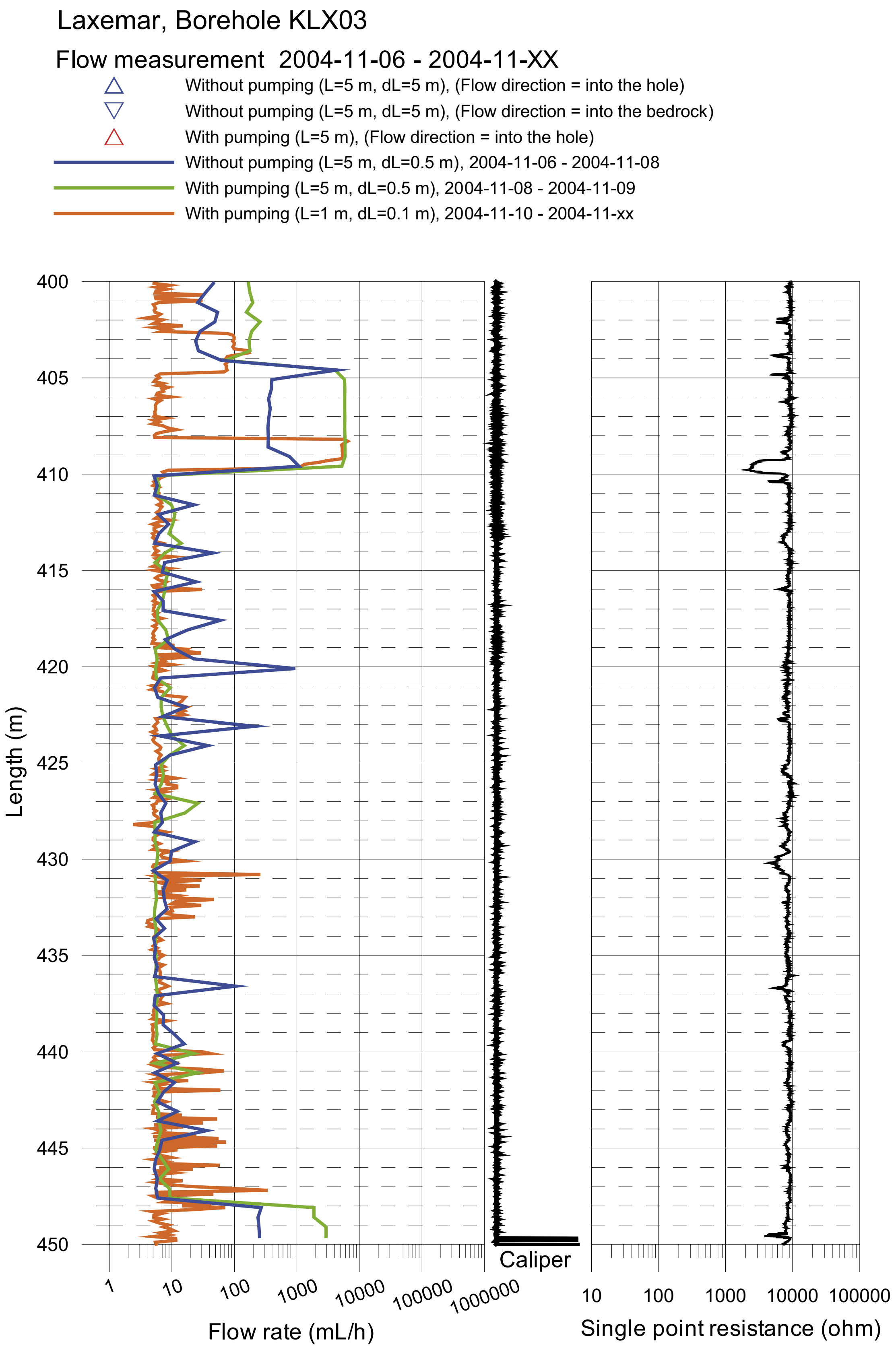


***Figure A2-2.** Borehole KLX03A: Differential flow measurements from 400–450 m including the water bearing fracture zone at approximately 410 m /6/.*

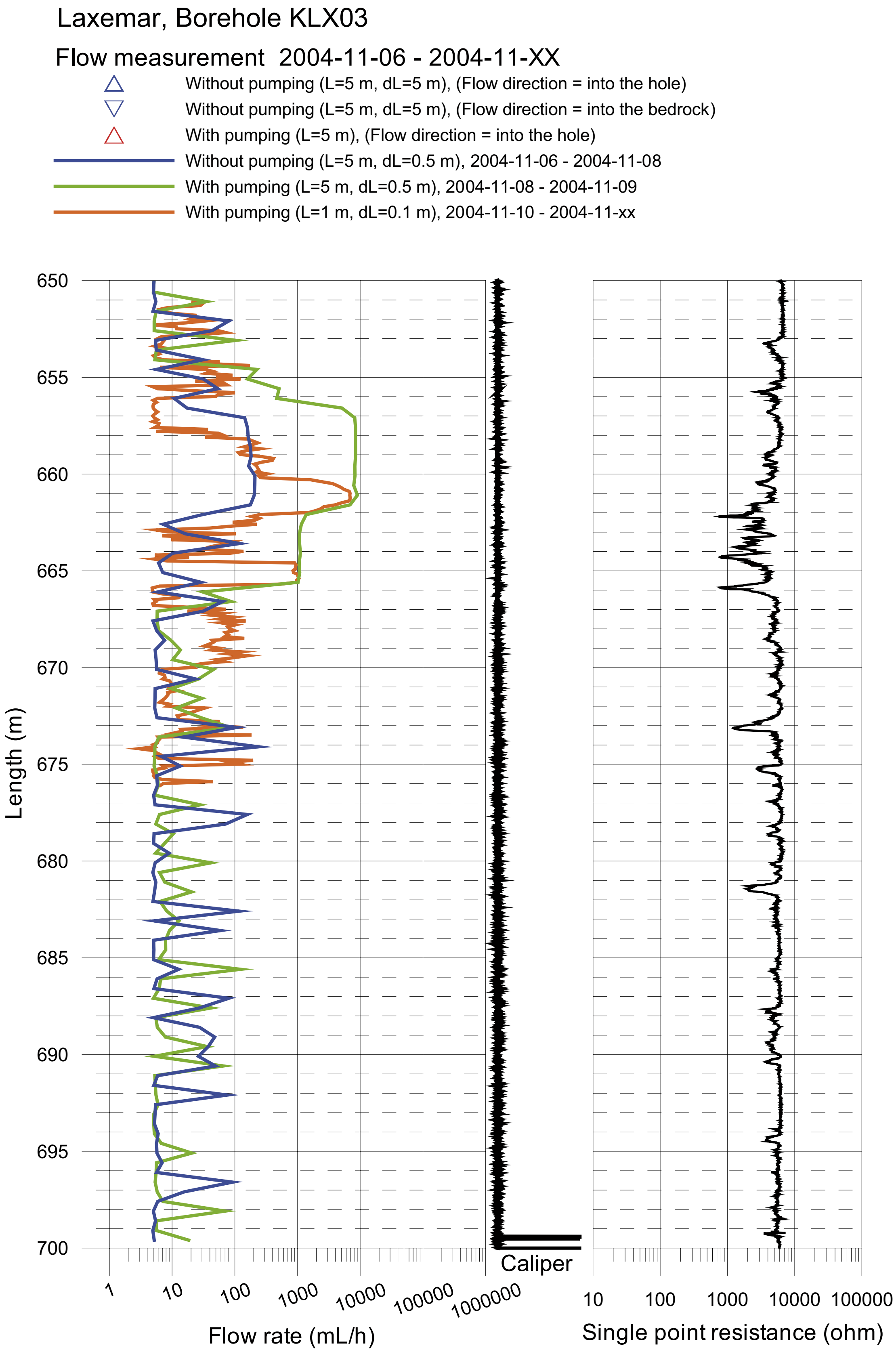


***Figure A2-3.** Borehole KLX03A: Differential flow measurements from 650–700 m including the water bearing fracture zone at approximately 662 m /6/.*

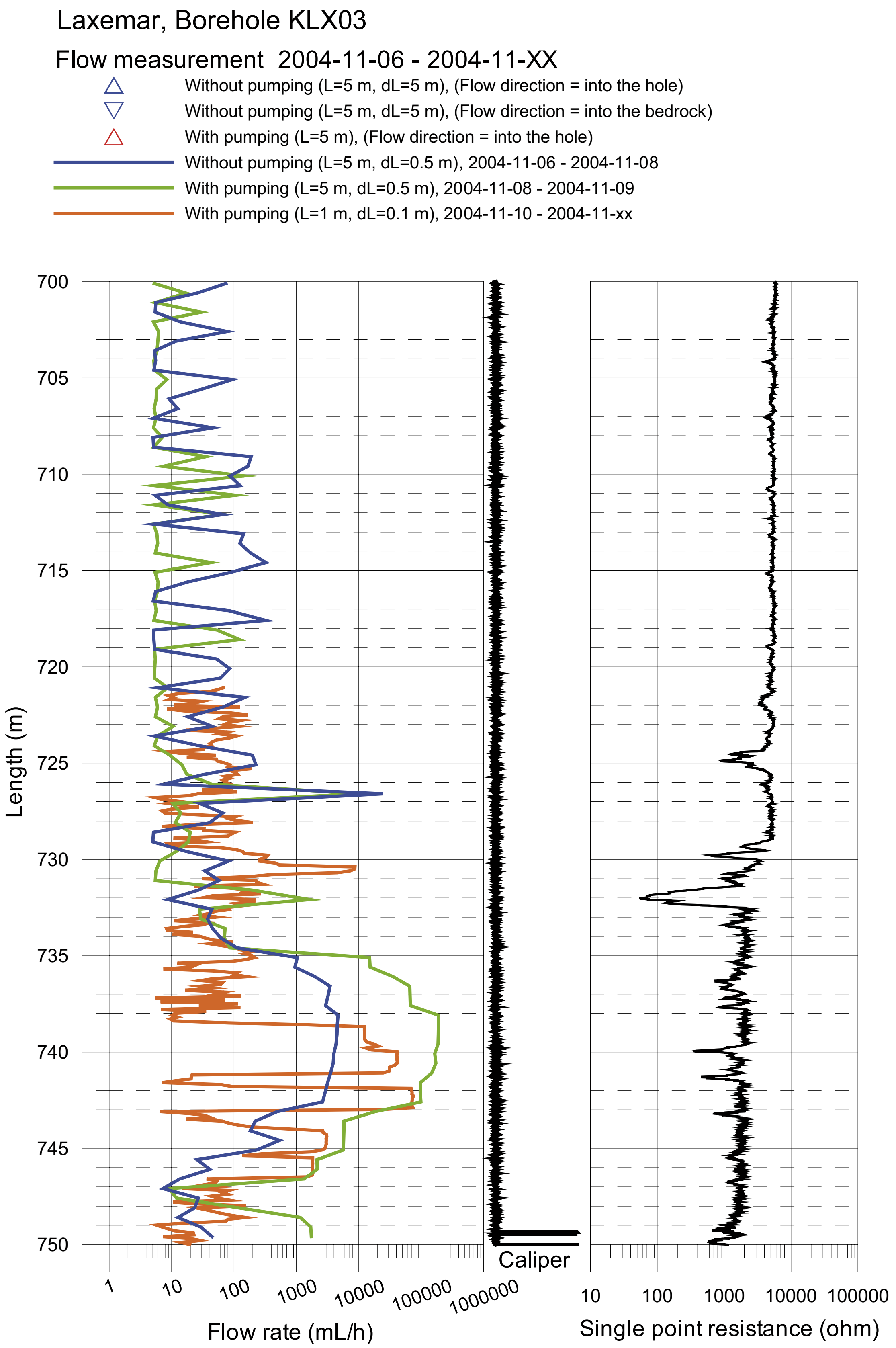


Figure A2-4. *Borehole KLX03A: Differential flow measurements from 700–750 m including the water bearing fracture zone at approximately 743 m /6/.*

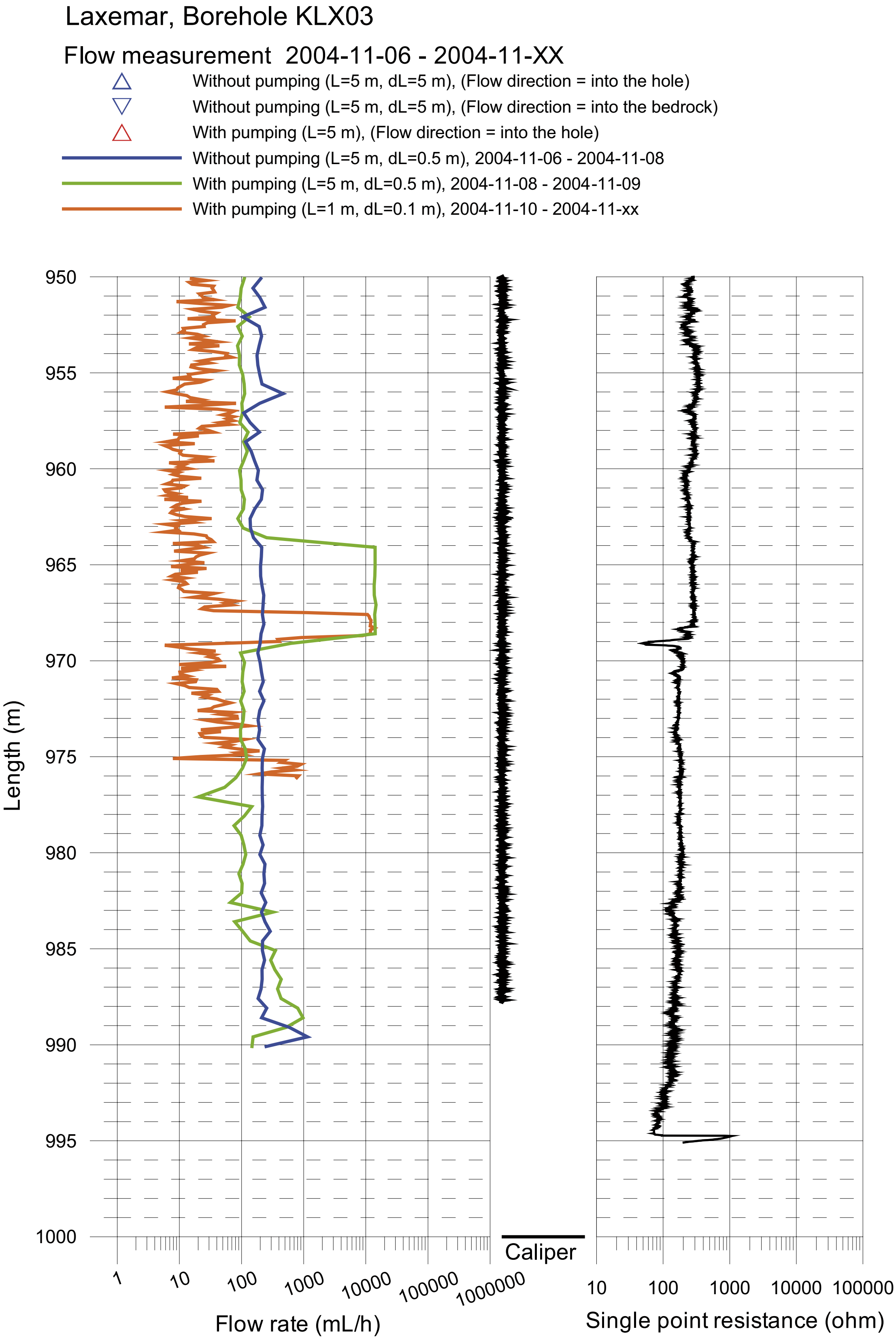
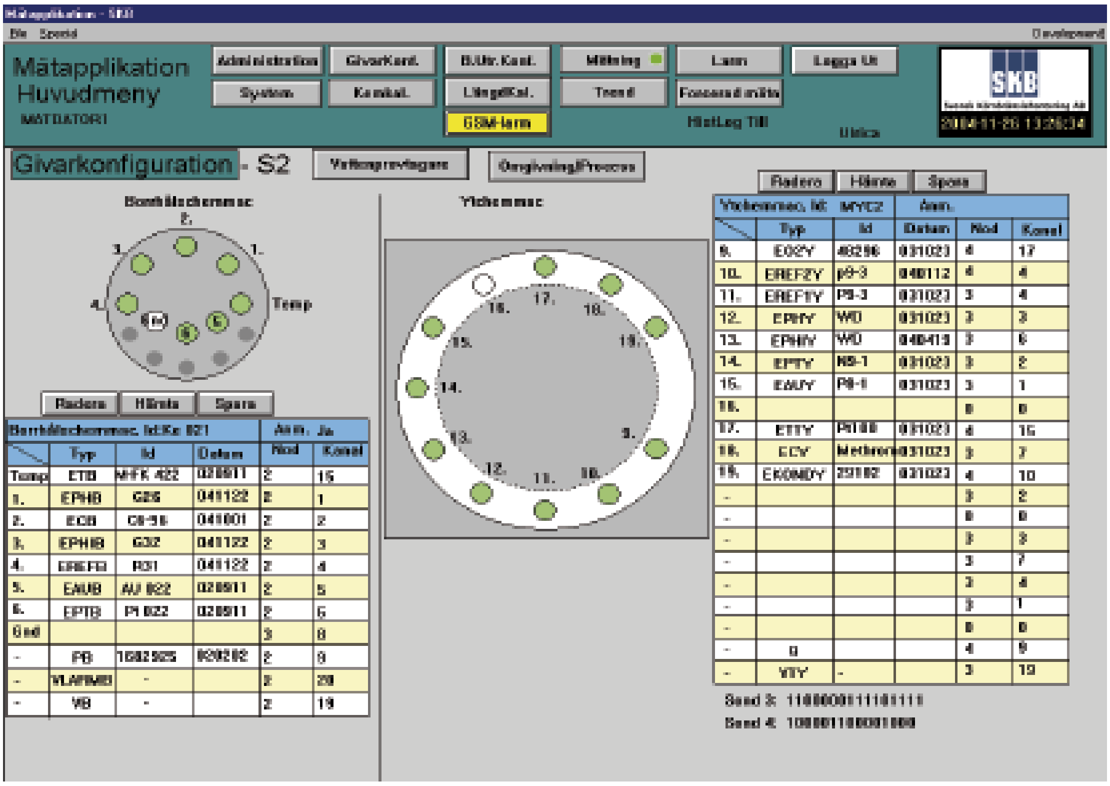


***Figure A2-5.** Borehole KLX03A: Differential flow measurements from 950–1,000 m including the water bearing fracture zone at approximately 969 m /6/.*

Appendix 3

Measurement information

Section 193.5–198.4 m



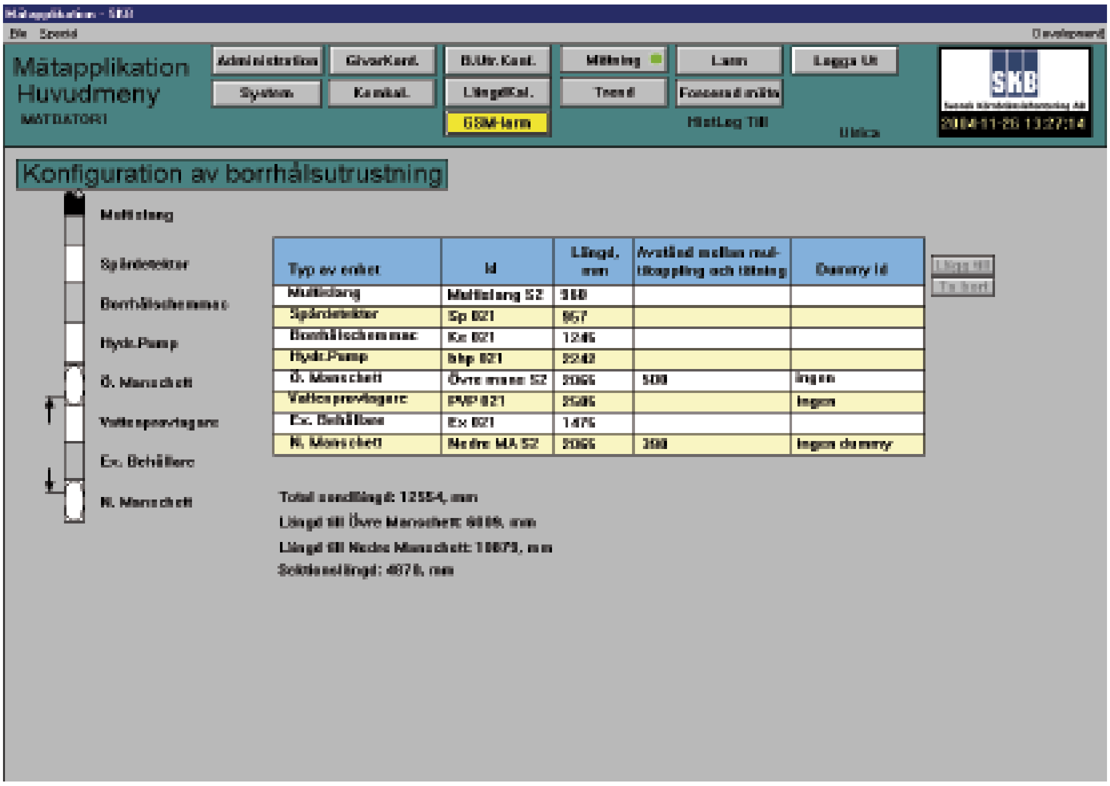
Borrhålsklemmar, Id:Kx 021				Anm. Ja	
	Typ	Id	Datum	Nod	Kanal
Temp	ETB	MFK 422	020911	2	15
1.	EPHB	G26	041122	2	1
2.	ECB	C8-58	041001	2	2
3.	EPHB	G32	041122	2	3
4.	EREFB	R31	041122	2	4
5.	EAUB	AU 022	020911	2	5
6.	EPTB	Pt 022	020911	2	6
Gnd				3	8
-	PB	1082525	020202	2	8
-	VLARMB	-		2	20
-	VB	-		2	19

Ytklemmar, Id: MYC2			Anm.		
	Typ	Id	Datum	Nod	Kanal
9.	EO2Y	40256	031023	4	17
10.	EREF2Y	p9-3	040112	4	4
11.	EREF1Y	P9-3	031023	3	4
12.	EPHY	WD	031023	3	3
13.	EPHY	WD	040419	3	6
14.	EPTY	N9-1	031023	3	2
15.	EAUY	P9-1	031023	3	1
16.				0	0
17.	ETTY	Pt100	031023	4	15
18.	ECY	Methrom	031023	3	7
19.	EKONDY	23102	031023	4	10
-				3	2
-				0	0
-				3	3
-				3	7
-				3	4
-				3	1
-				0	0
-	Q			4	9
-	VTY	-		3	19

Send 3: 1100000111101111

Send 4: 1000011000001000

Figure A3-1. Electrode configuration, section 193.5–198.4 m.



Typ av enhet	Id	Längd, mm	Avstånd mellan multikoppling och tätning	Dummy id
Multislang	Multislang S2	380		
Spårdetektor	Sp 021	957		
Borrhålsklemmar	Kx 021	1246		
Hydr.Pump	hhp 021	2242		
Ö. Manschett	Övre mans S2	2066	500	Ingen
Vattenprovtagare	PVP 021	2505		Ingen
Ex. Behållare	Ex 021	1476		
N. Manschett	Nedre MA S2	2066	300	Ingen dummy

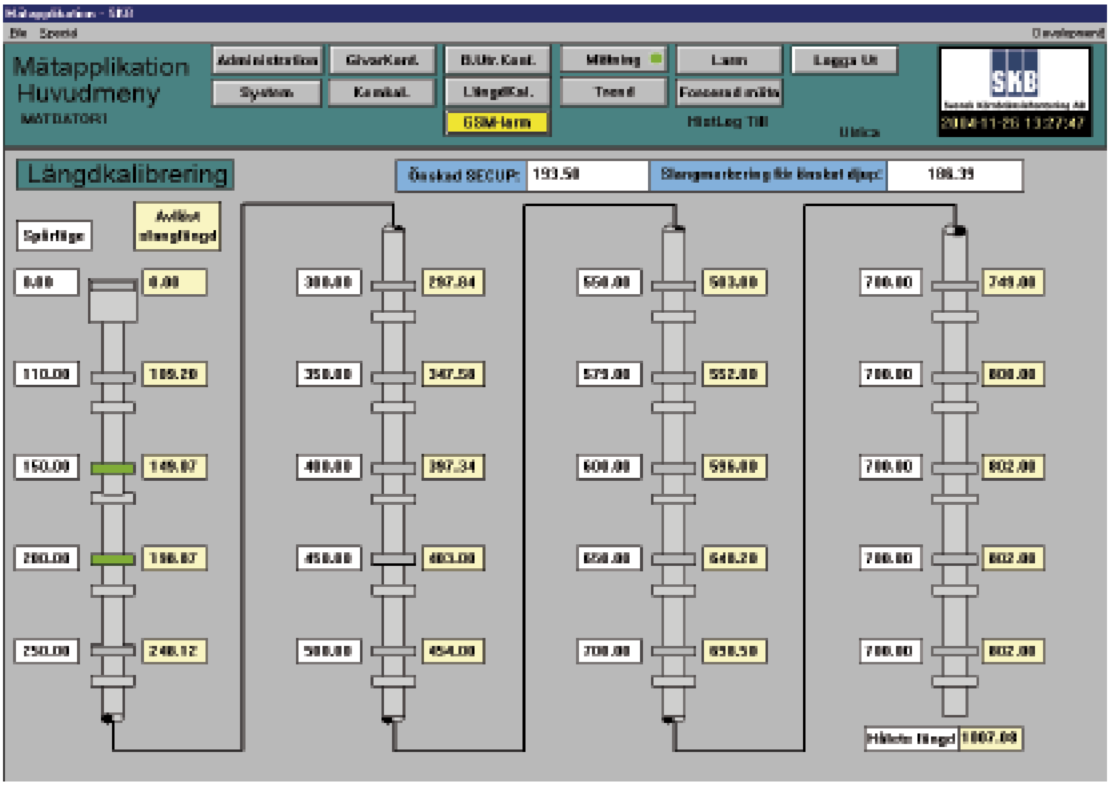
Total sondlängd: 12554, mm

Längd till Övre Manschett: 6009, mm

Längd till Nedre Manschett: 10879, mm

Sektionslängd: 4870, mm

Figure A3-2. Configuration of downhole equipment, section 193.5–198.4 m.



Önskad SECUP: 193.50

Slangmarkering för önskat djup: 198.39

Spårlängd	Avläst slanglängd
0.00	0.00
110.00	109.20
150.00	149.07
200.00	198.07
250.00	248.12
300.00	297.84
350.00	347.58
400.00	397.34
450.00	403.00
500.00	454.00
550.00	503.00
575.00	552.00
600.00	596.00
650.00	640.20
700.00	650.50
700.00	749.00
700.00	800.00
700.00	802.00
700.00	802.00
700.00	802.00

Hämta längd 1007.00

Figure A3-3. Length calibration, section 193.5–198.4 m.

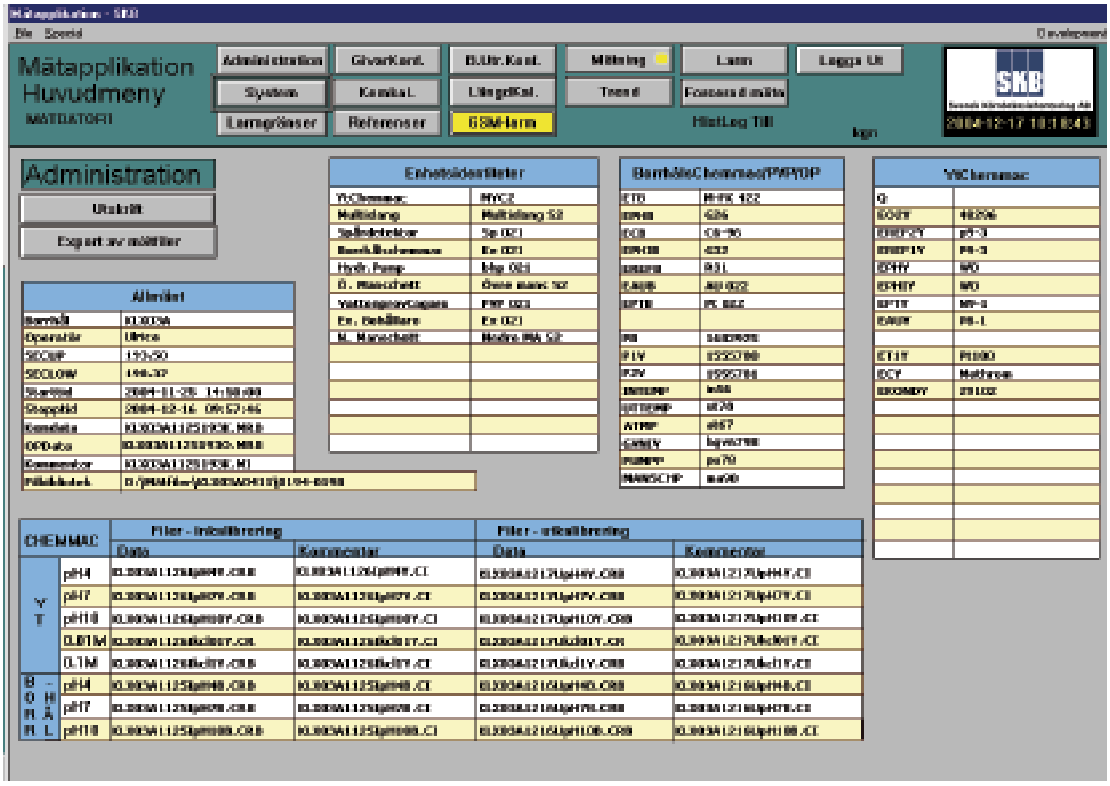
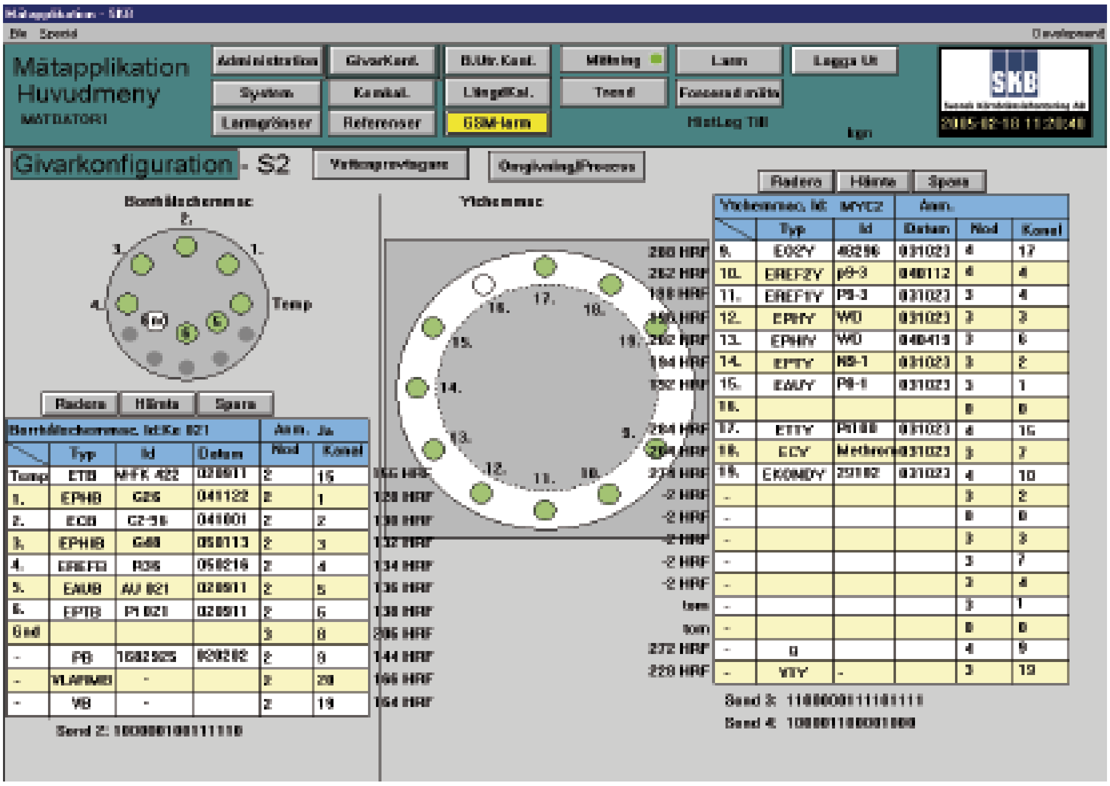


Figure A3-4. Administration, section 193.5–198.4 m.

Section 408.0–415.3 m



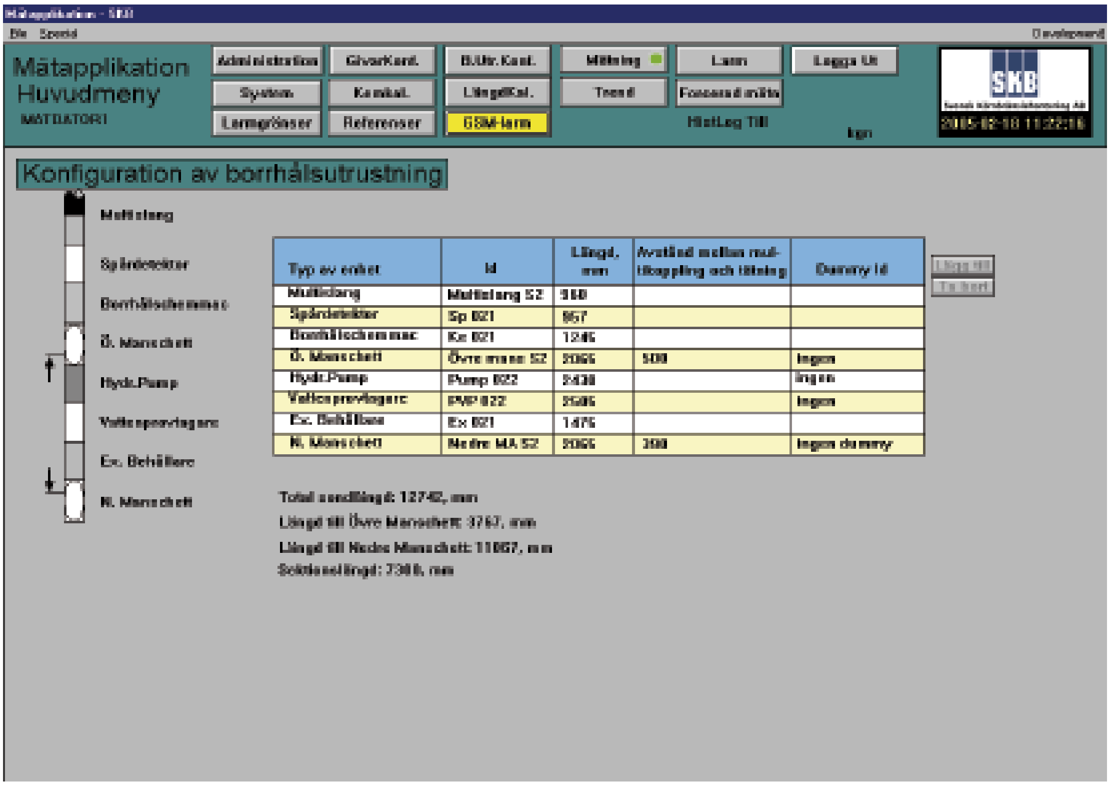
Borrhålschemmac. Id:Ks 021				Ann. Ja	
	Typ	Id	Datum	Nod	Kanal
Temp	ETB	MFK 422	020911	2	15
1.	EPHB	G26	041122	2	1
2.	ECB	C2-98	041001	2	2
3.	EPHB	G48	050113	2	3
4.	EREFB	R36	050216	2	4
5.	EAUB	AU 021	020911	2	5
6.	EPTB	Pt 021	020911	2	6
Gnd				3	0
-	PB	1082925	020202	2	9
-	VLAPMB	-		2	20
-	VB	-		2	19

Send 2: 1000001000111110

Ytchemmac. Id: MYC2			Ann.		
	Typ	Id	Datum	Nod	Kanal
9.	EO2Y	40290	031023	4	17
10.	EREF2Y	p9-3	040112	4	4
11.	EREF1Y	P8-3	031023	3	4
12.	EPHY	WD	031023	3	3
13.	EPHY	WD	040419	3	6
14.	EPTY	N8-1	031023	3	2
15.	EAUY	P8-1	031023	3	1
16.				0	0
17.	ETTY	Pt100	031023	4	16
18.	ECY	Methrom	031023	3	7
19.	EKONDY	29102	031023	4	10
-				3	2
-				0	0
-				3	3
-				3	7
-				3	4
-				3	1
-				0	0
-	0			4	9
-	YTY	-		3	13

Send 3: 1100000111101111
Send 4: 1000011000001000

__Figure A3-5.__ Electrode configuration, section 408.0–415.3 m.



Typ av enhet	Id	Längd, mm	Avstånd mellan nollkoppling och tätning	Dummy Id
Multislang	Multislang S2	980		
Spårdetektor	Sp 021	857		
Borrhålschemmac	Ks 021	1246		
Ö. Manschett	Övre mans S2	2066	500	Ingen
Hydr.Pump	Pump 022	2438		Ingen
Vattenprovtagare	PVP 022	2586		Ingen
Ex. Behållare	Ex 021	1476		
N. Manschett	Nedre MA S2	2066	300	Ingen dummy

Total sondlängd: 12742, mm
Längd till Övre Manschett: 3767, mm
Längd till Nedre Manschett: 11067, mm
Sektionslängd: 7300, mm

__Figure A3-6.__ Configuration of downhole equipment, section 408.0–415.3 m.

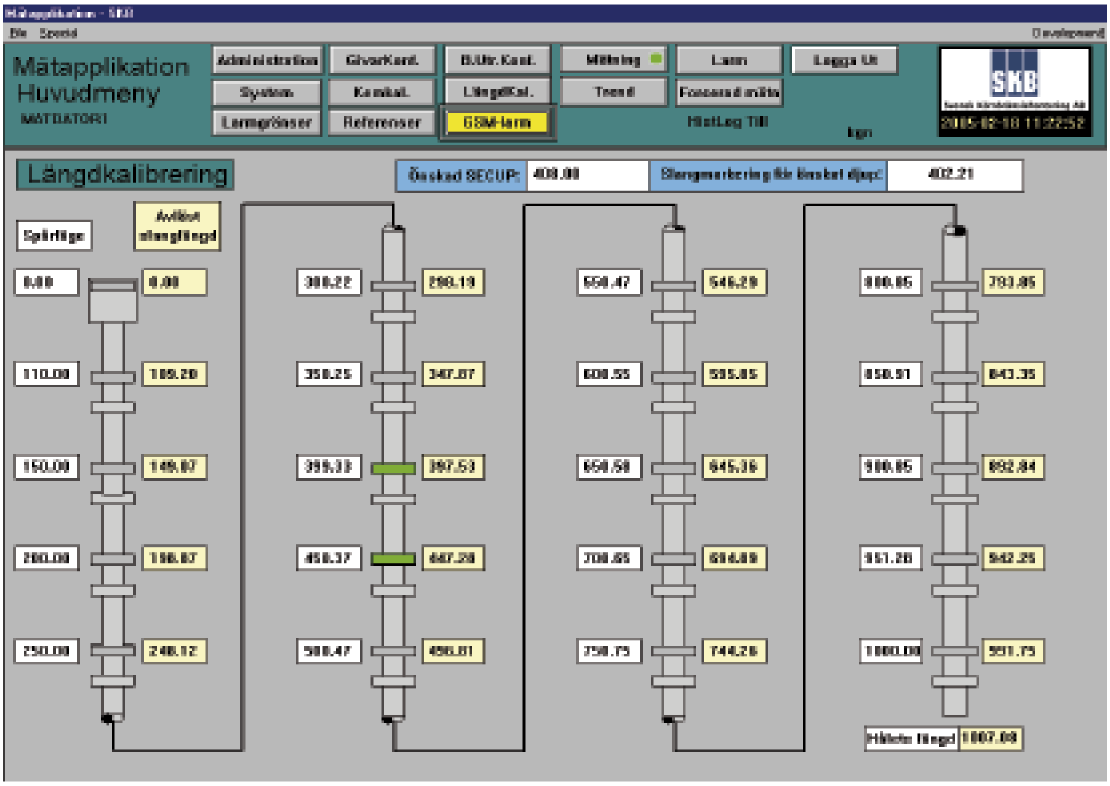


Figure A3-7. *Length calibration, section 408.0–415.3 m.*

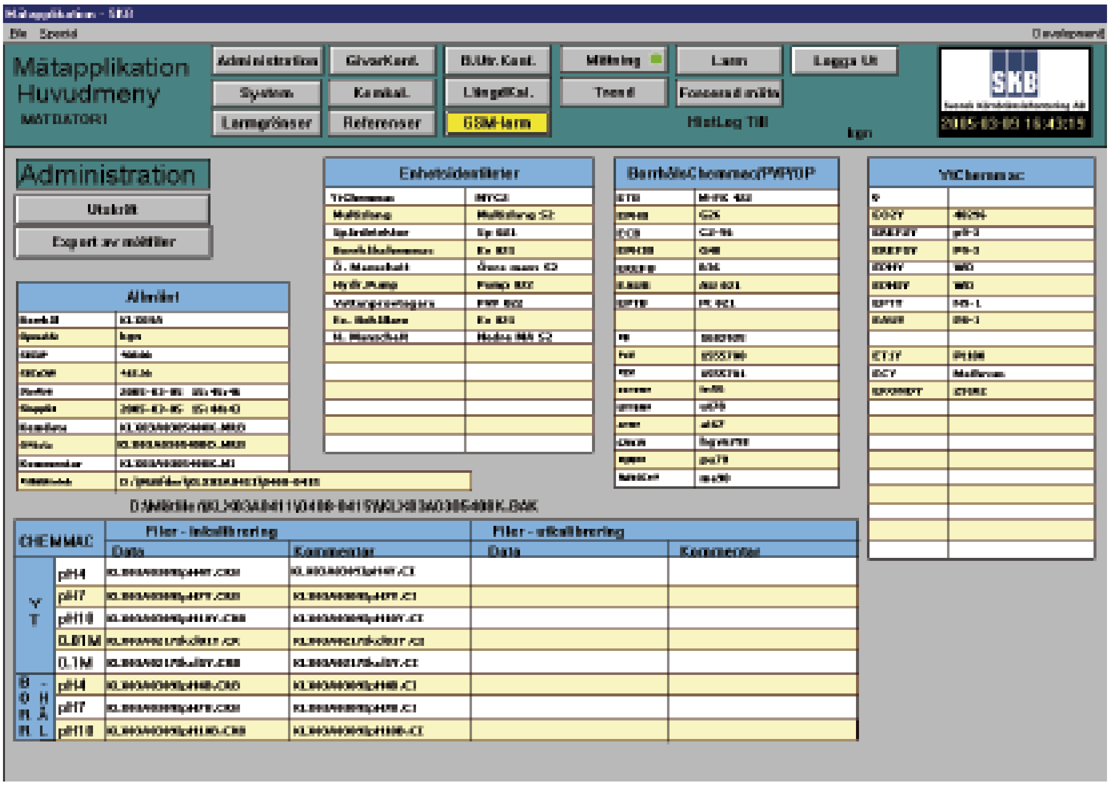
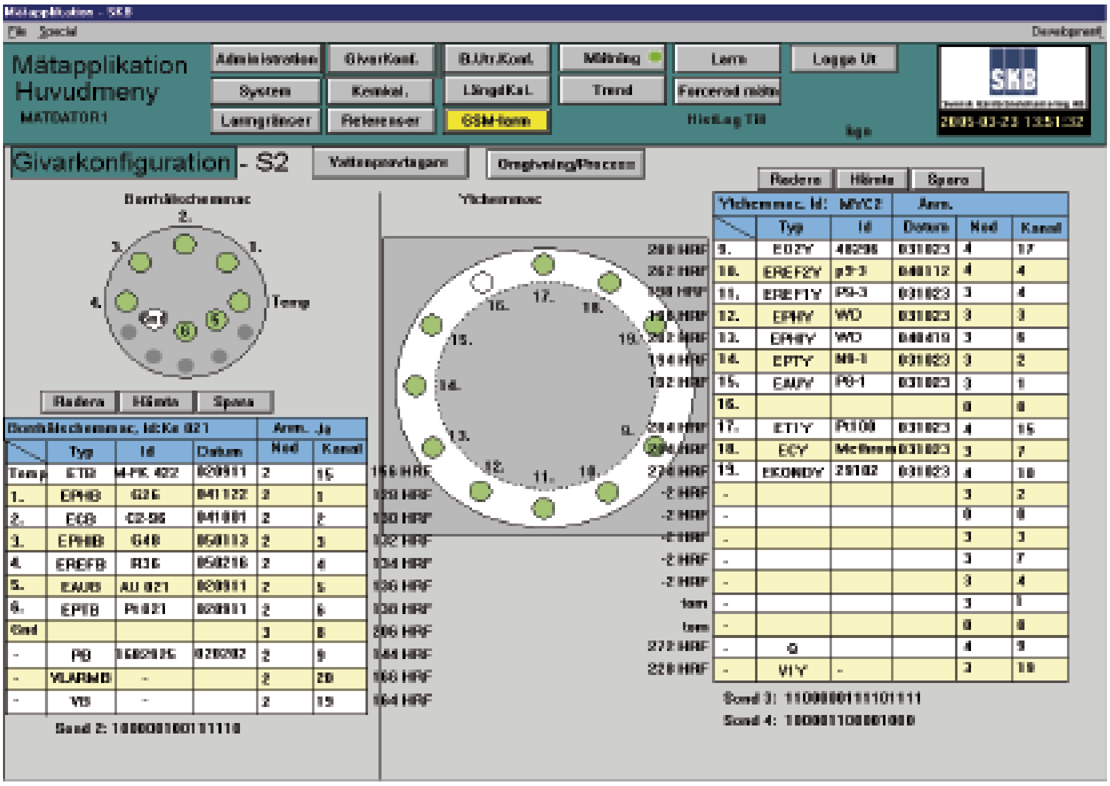


Figure A3-8. *Administration, section 408.0–415.3 m.*

Section 735.5–748.0 m



Borrhålsschemmac, Id:Ka 021				Arm. Ja	
	Typ	Id	Datum	Nod	Kanal
Temp	ETG	M-PK 422	020911	2	15
1.	EPHB	G26	041122	2	1
2.	ECB	C2-96	041001	2	2
3.	EPHB	G48	050113	2	3
4.	EREFB	R36	050216	2	4
5.	EAUB	AU 021	020911	2	5
6.	EPTB	Pt 021	020911	2	6
Gnd				3	8
-	PB	16602026	020202	2	9
-	VLARMB	-		2	20
-	VB	-		2	19

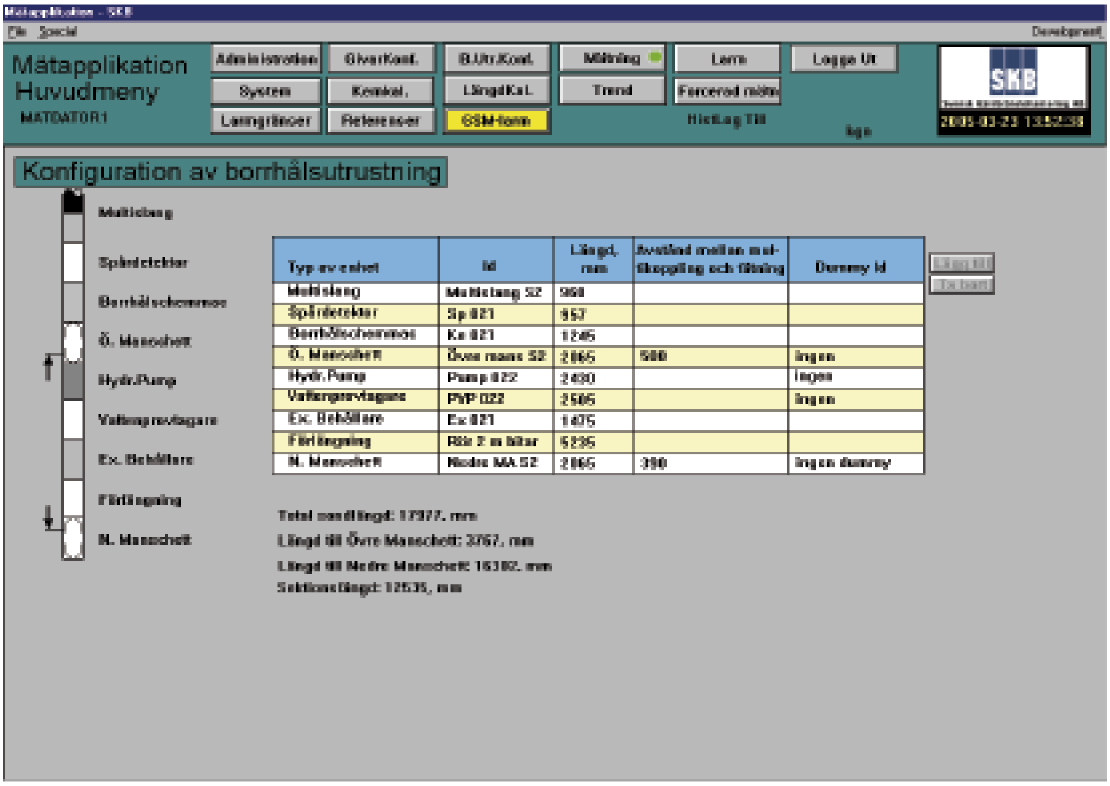
Sond 2: 1000001001111110

Ytschemmac. Id: MYC2			Arm.		
	Typ	Id	Datum	Nod	Kanal
9.	EOZY	40298	031023	4	17
10.	EREF2Y	p9-3	040112	4	4
11.	EREF1Y	P9-3	031023	3	4
12.	EPHY	WD	031023	3	3
13.	EPHY	WD	040419	3	6
14.	EPTY	M8-1	031023	3	2
15.	EAUY	P8-1	031023	3	1
16.				0	0
17.	ETIY	Pt100	031023	4	15
18.	ECY	Meltem	031023	3	7
19.	EKONDY	28102	031023	4	10
-				3	2
-				0	0
-				3	3
-				3	7
-				3	4
-				3	1
-				0	0
-	Q			4	9
-	VIY	-		3	10

Sond 3: 1100000111101111

Sond 4: 1000011000001000

Figure A3-9. *Electrode configuration, section 735.5–748.0 m.*



Typ av enhet	Id	Längd, mm	Avstånd mellan mä-tkoppling och tätning	Dummy Id
Multislang	Multislang S2	960		
Spårdetektor	Sp 021	957		
Borrhålsschemmac	Ka 021	1245		
Ö. Manschett	Övre mans S2	2065	500	ingen
Hydr.Pump	Pump 022	2490		ingen
Vattenprovtagare	PVP 022	2505		ingen
Ex. Behållare	Ex 021	1475		
Förlängning	Rör 2 m bitar	5235		
N. Manschett	Nedre MA S2	2065	390	ingen dummy

Total sondlängd: 17977, mm

Längd till Övre Manschett: 3767, mm

Längd till Nedre Manschett: 16302, mm

Sektionslängd: 12535, mm

Figure A3-10. *Configuration of downhole equipment, section 735.5–748.0 m.*

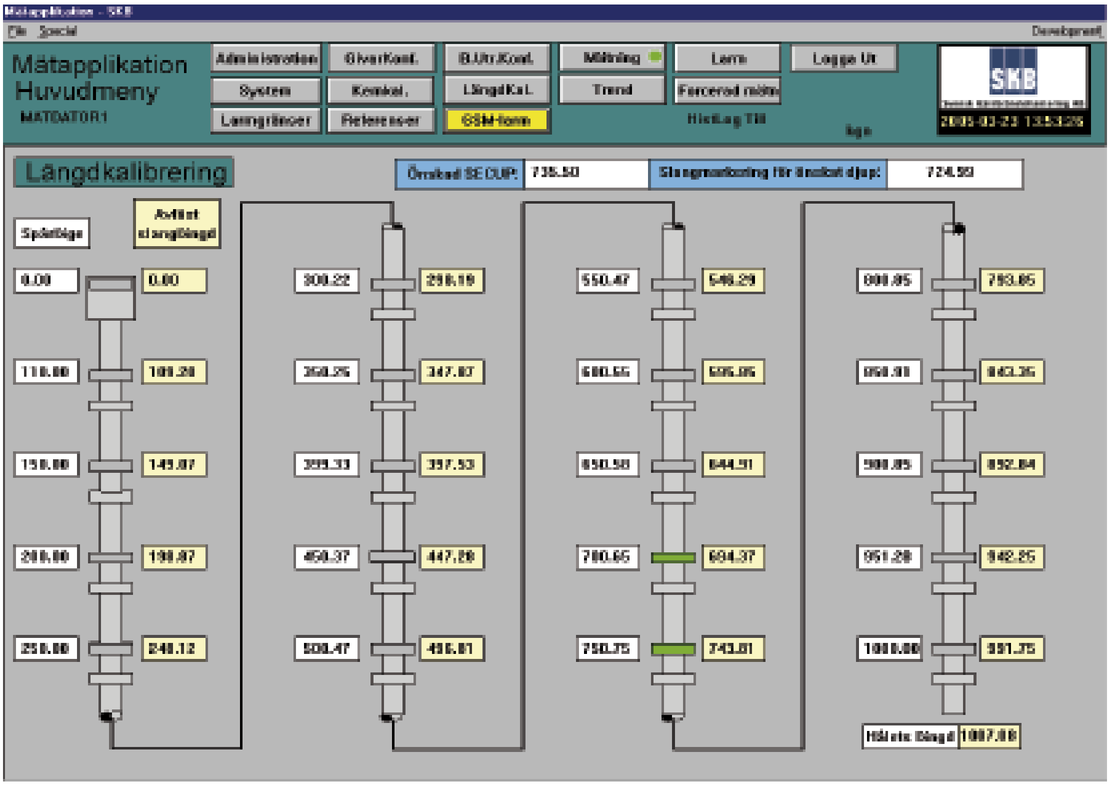


Figure A3-11. *Length calibration, section 735.5–748.0 m.*

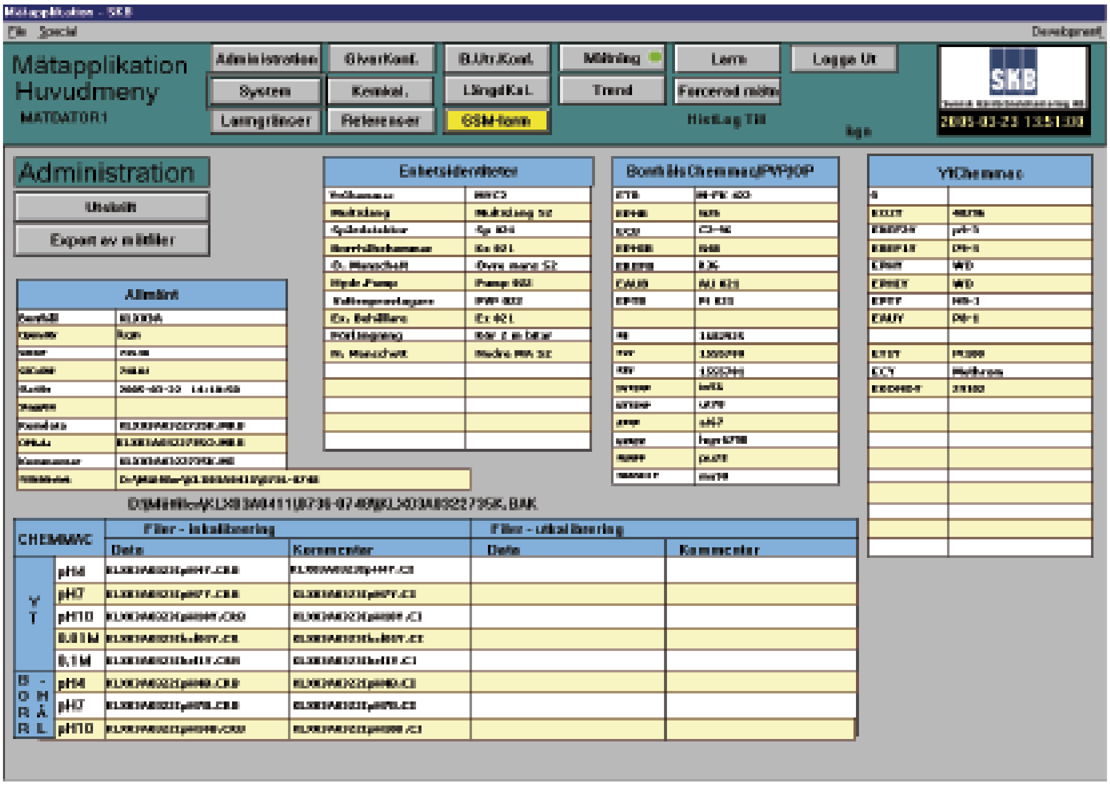
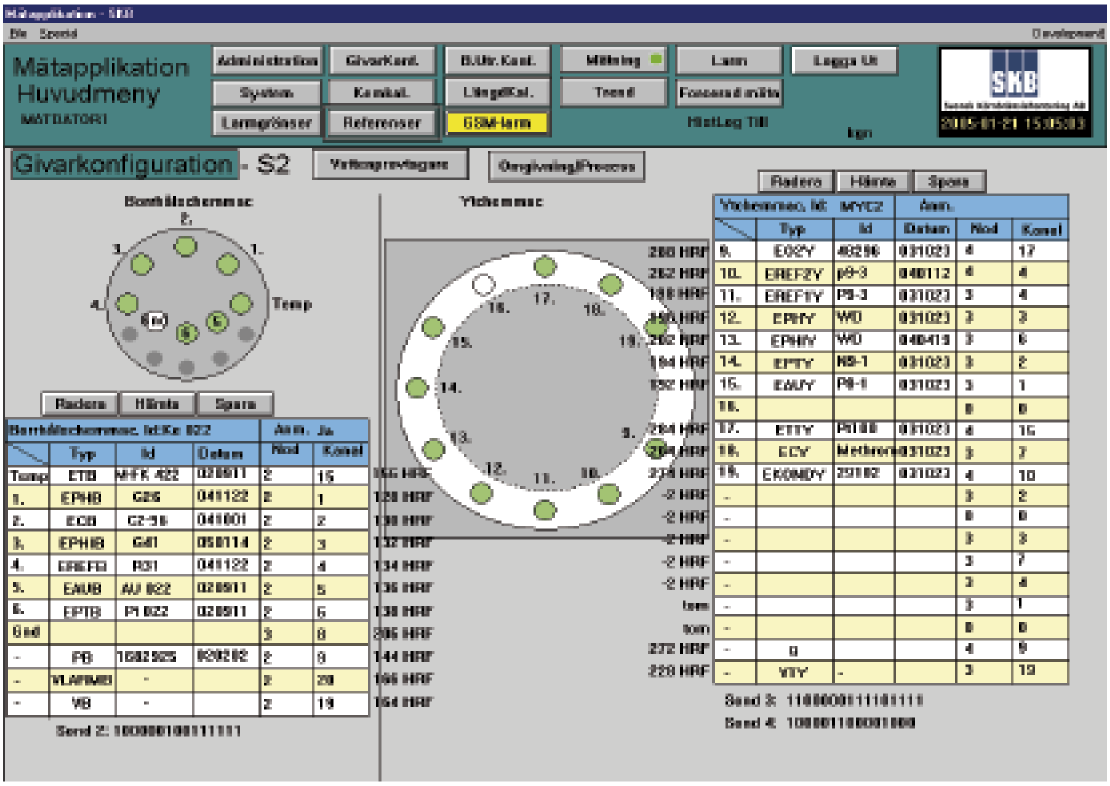


Figure A3-12. *Administration, section 735.5–748.0 m.*

Section 964.5–975.2 m



Borrhålschemmac. Id:Ks 022				Ann. Ja	
	Typ	Id	Datum	Nod	Kanal
Temp	ETB	MFK 422	020911	2	15
1.	EPHB	G26	041122	2	1
2.	ECB	G2-38	041001	2	2
3.	EPHB	G41	050114	2	3
4.	EREFB	R31	041122	2	4
5.	EAUB	AU 022	020911	2	5
6.	EPTB	Pt 022	020911	2	6
Gnd				3	8
-	PB	1082925	020202	2	9
-	VLARMB	-		2	20
-	VB	-		2	19

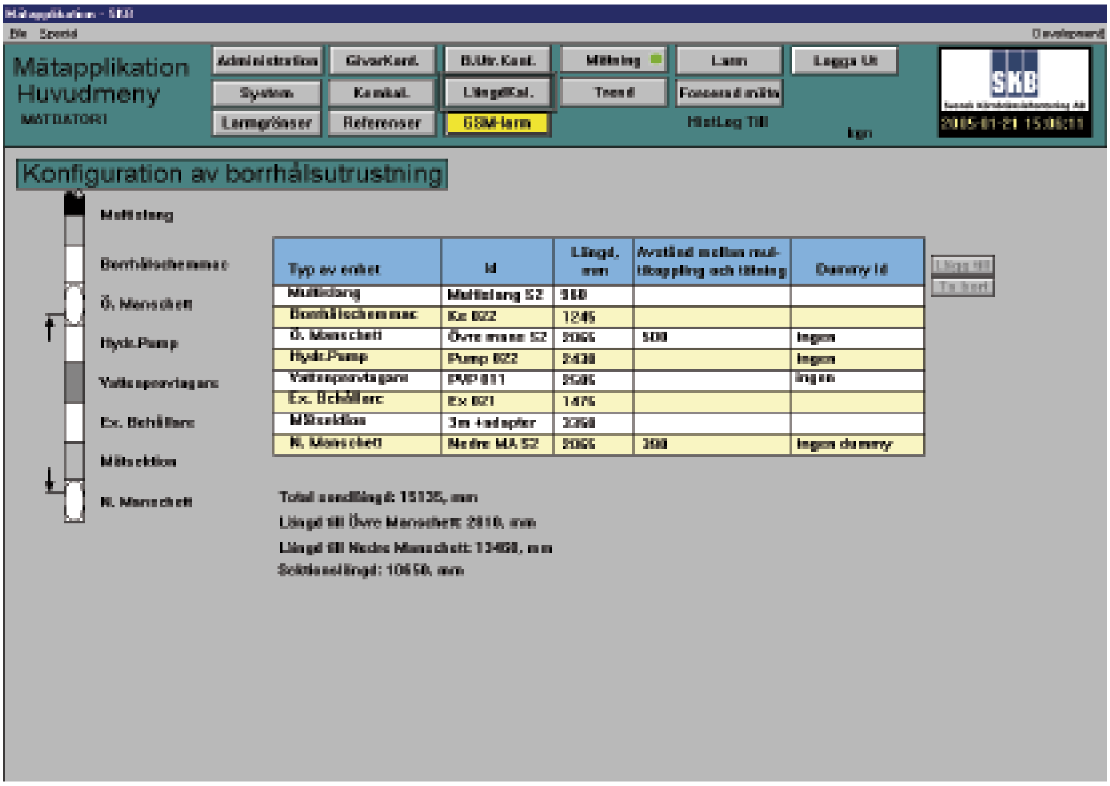
Send 2: 1000000100111111

Ytchemmac. Id: MYC2			Ann.		
	Typ	Id	Datum	Nod	Kanal
9.	EO2Y	40290	031023	4	17
10.	EREF2Y	p9-3	040112	4	4
11.	EREF1Y	P9-3	031023	3	4
12.	EPHY	WD	031023	3	3
13.	EPHY	WD	040419	3	6
14.	EPTY	N9-1	031023	3	2
15.	EAUY	P9-1	031023	3	1
16.				0	0
17.	ETTY	Pt100	031023	4	16
18.	ECY	Methrom	031023	3	7
19.	EKONDY	29102	031023	4	10
-				3	2
-				0	0
-				3	3
-				3	7
-				3	4
-				3	1
-				0	0
-	0			4	9
-	VTY	-		3	19

Send 3: 1100000111101111

Send 4: 1000011000001000

Figure A3-13. Electrode configuration, section 964.5–975.2 m.



Konfiguration av borrhålsutrustning

Typ av enhet	Id	Längd, mm	Avstånd mellan nul-tikoppling och tätning	Dummy Id
Multislang	Multislang S2	960		
Borrhålschemmac	Ks 022	1245		
Ö. Manschett	Övre mans S2	2065	500	Ingen
Hydr.Pump	Pump 022	2430		Ingen
Vattenprovtagare	PVP 011	2505		Ingen
Ex. Behållare	Ex 021	1475		
Mätsektion	3m +adapter	3350		
N. Manschett	Nedre MA S2	2065	300	Ingen dummy

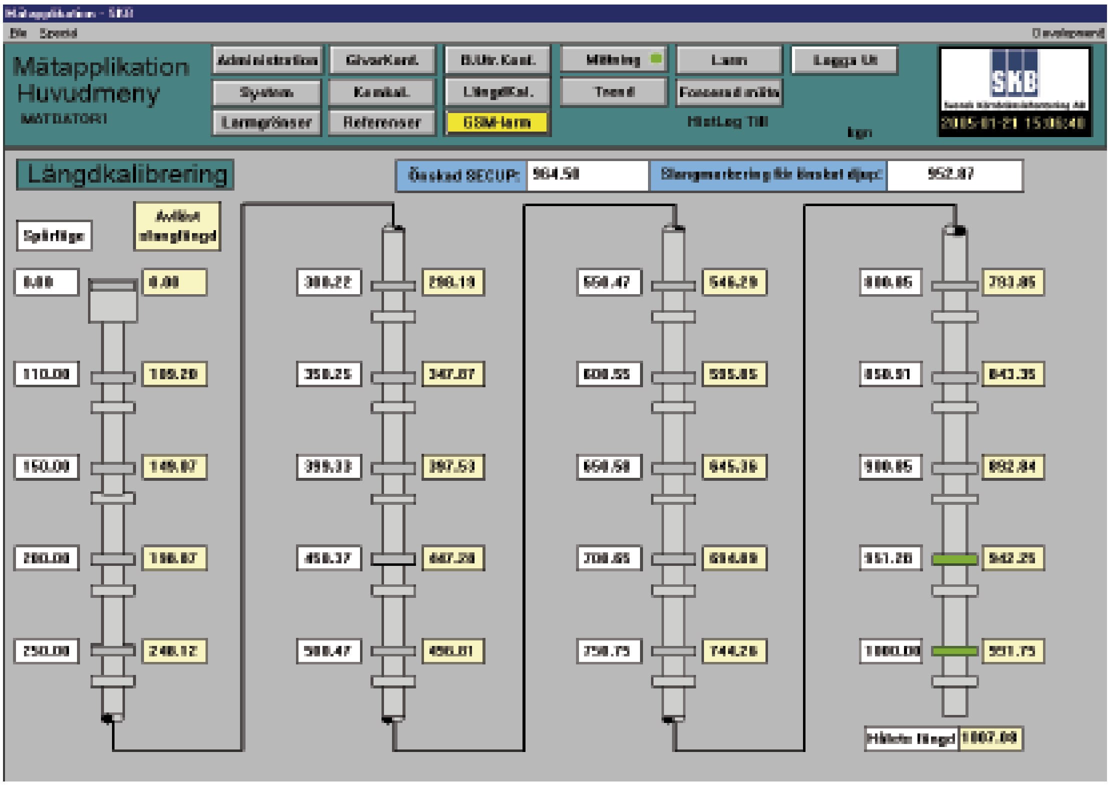
Total sondlängd: 15135, mm

Längd till Övre Manschett: 2810, mm

Längd till Nedre Manschett: 13460, mm

Sektionslängd: 10650, mm

Figure A3-14. Configuration of downhole equipment, section 964.5–975.2 m.



Spårlänge	Avläst slanglängd
0.00	0.00
110.00	109.20
150.00	149.07
200.00	198.87
250.00	248.12
300.22	298.19
350.25	347.87
399.33	397.53
450.37	447.28
500.47	496.81
550.47	546.29
600.55	595.85
650.58	645.36
700.65	694.89
750.75	744.20
800.85	793.85
850.91	843.35
900.85	892.84
951.20	942.25
1000.00	991.75

Figure A3-15. *Length calibration, section 964.5–975.2 m.*

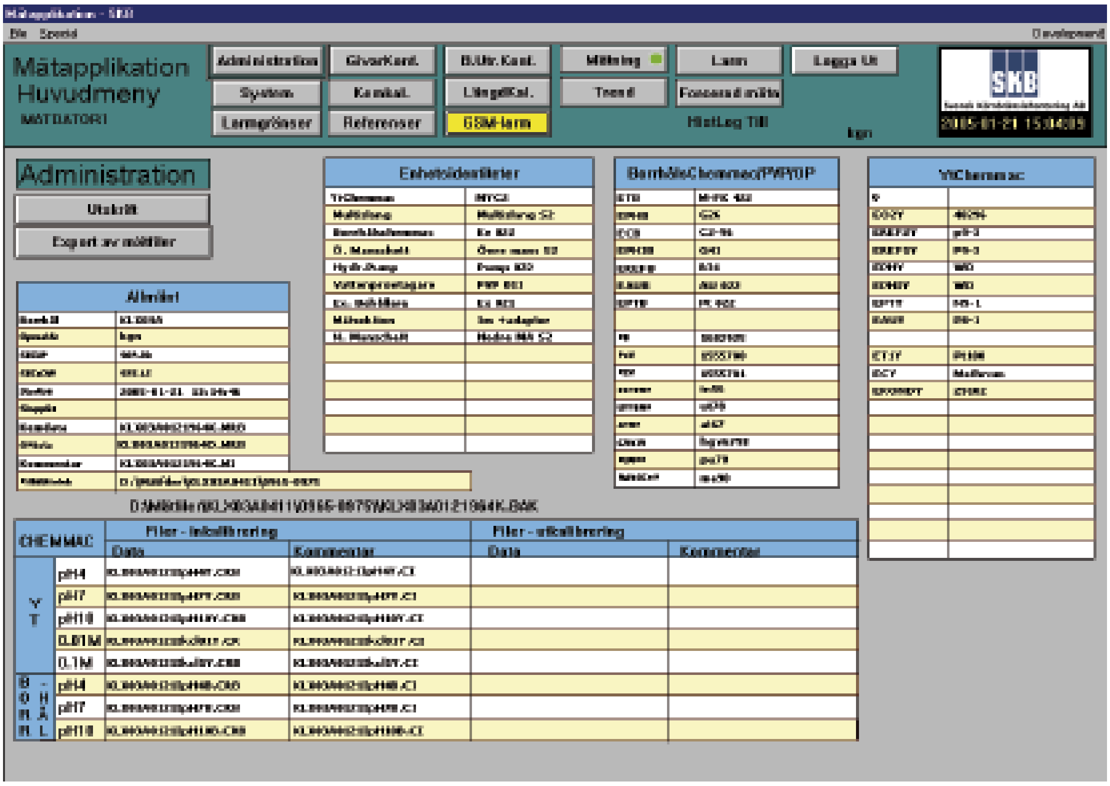


Figure A3-16. *Administration, section 964.5–975.2 m.*

Appendix 4

Flow and pressure measurements

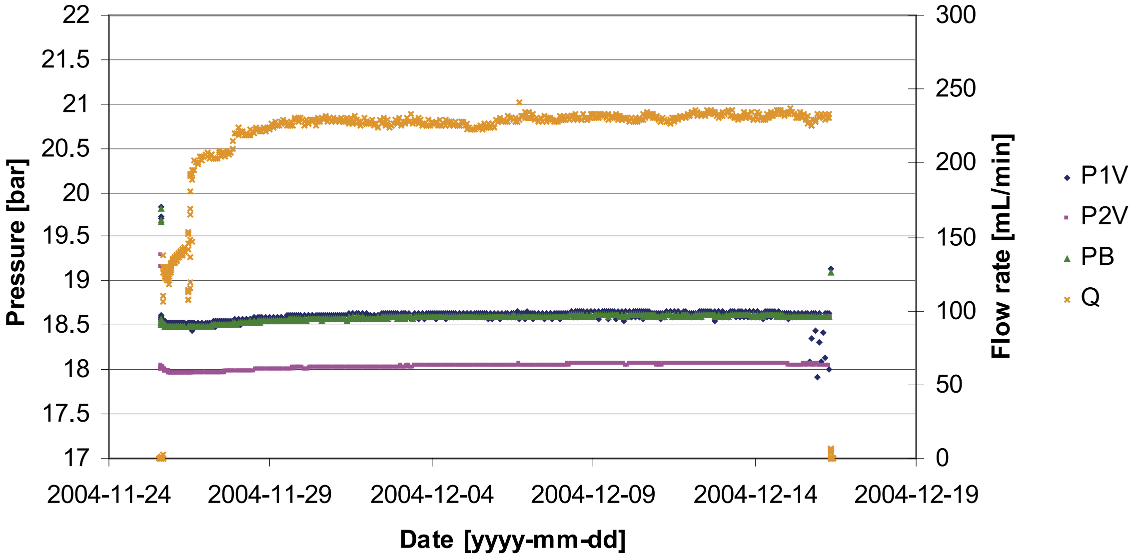


Figure A4-1. Pressure (P1V, P2V and PB) and flow rate (Q) measurements in borehole section 193.5–198.4 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. PB is the sensor in the borehole chemmac and measures the pressure above the section.

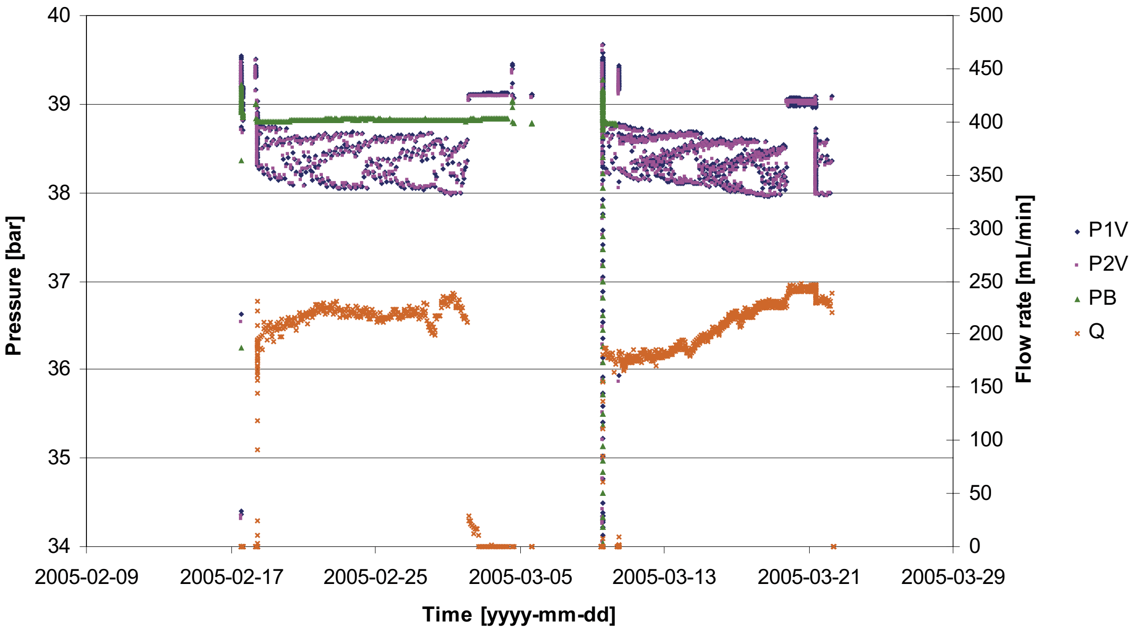


Figure A4-2. Pressure (P1V, P2V and PB) and flow rate (Q) measurements in borehole section 408.0–415.3 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. PB is the sensor in the borehole chemmac and measures the pressure above the section. March 10:th the PB sensor ceased to function and no PB measurements are available after that time.

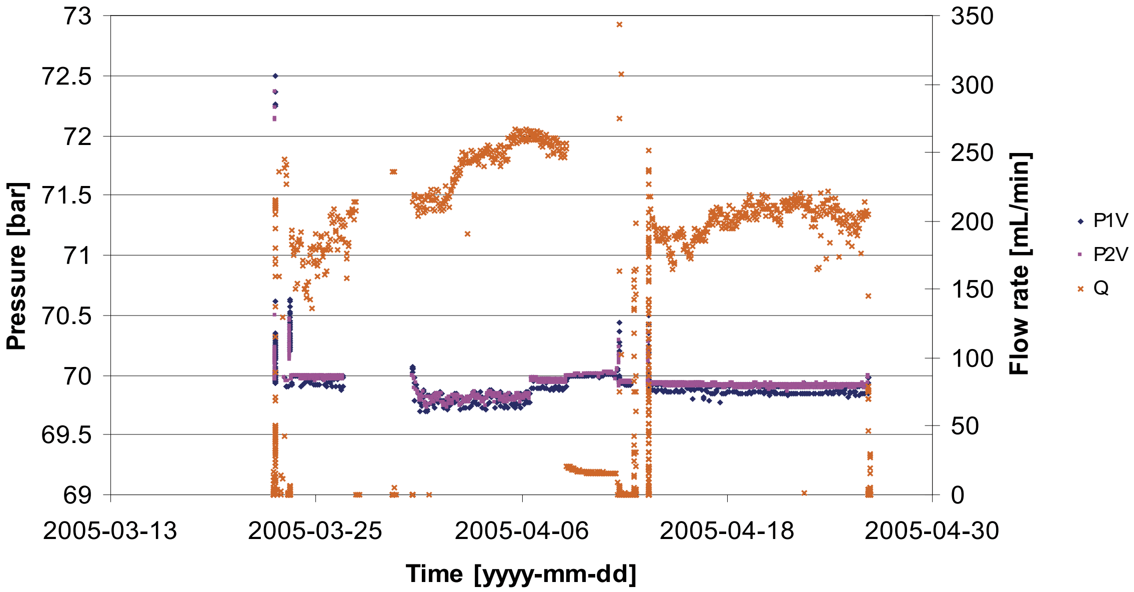


__Figure A4-3.__ Pressure (P1V, P2V) and flow rate (Q) measurements in borehole section 735.5–748.0 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. The PB sensor in the borehole chemmac (measuring the pressure above the section) was out of order during the investigation.

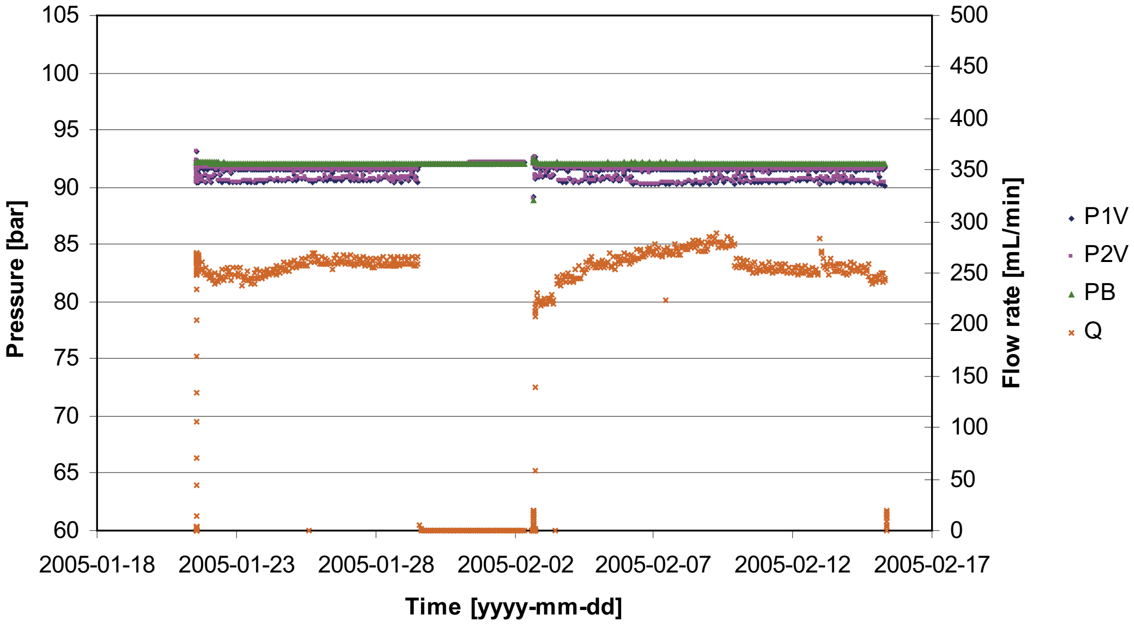


__Figure A4-4.__ Pressure (P1V, P2V and PB) and flow rate (Q) measurements in borehole section 964.5–975.2 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. PB is the sensor in the borehole chemmac and measures the pressure above the section.

Appendix 5

Chemmac measurements (Eh, pH, electrical conductivity, dissolved oxygen and temperature) section 193.5–198.4 m

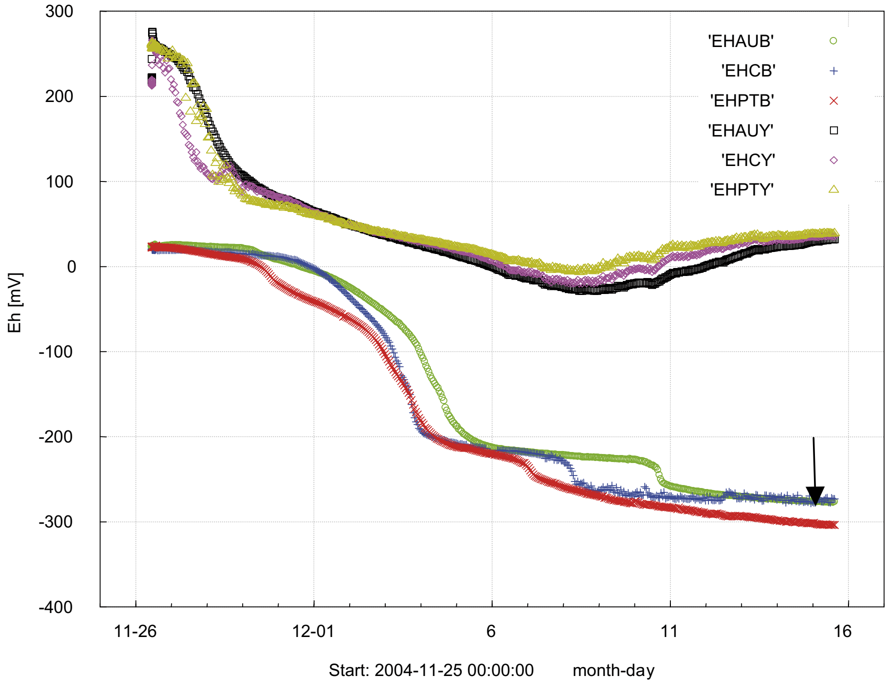


Figure A5-1. Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.

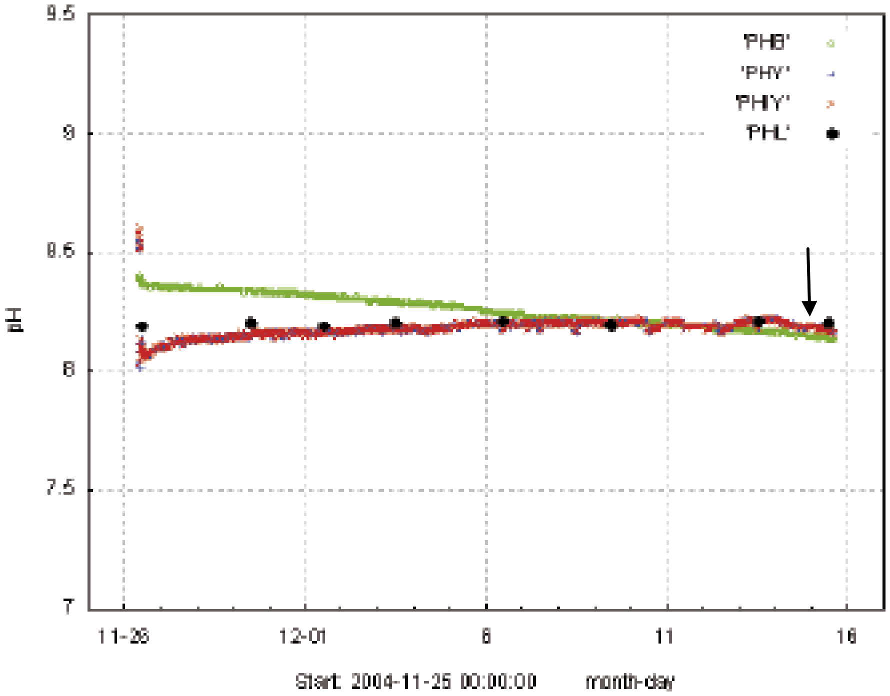


Figure A5-2. Measurements of pH by one glass electrodes in the borehole section (PHB) and two glass electrode at the surface (PHY and PHIY). The response from PHIB was not stable and was therefore rejected. The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.

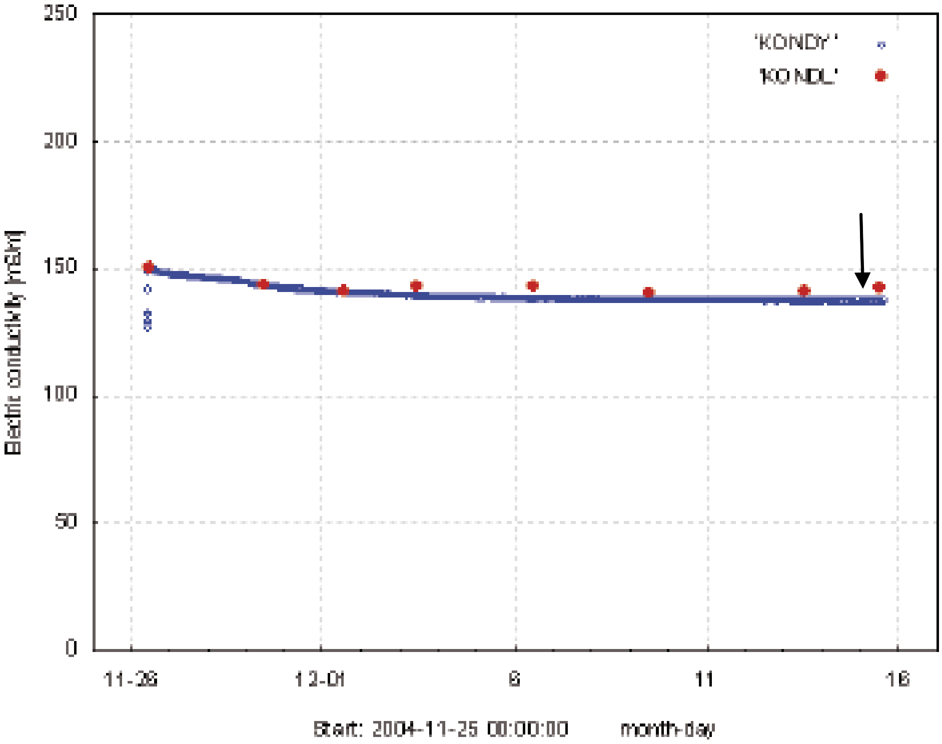


Figure A5-3. *Electrical conductivity measurement in the surface measurement cell (KONDY). The laboratory conductivity in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.*

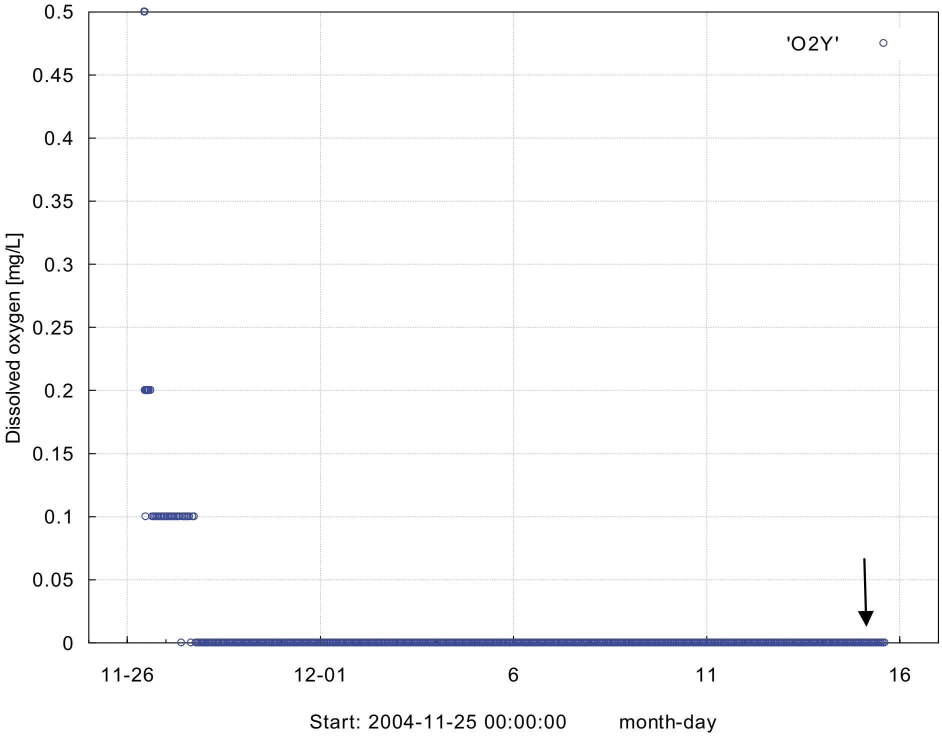


Figure A5-4. *Dissolved oxygen measurement (O2Y) in the surface measurement cell. The arrow shows the chosen representative value for dissolved oxygen in the borehole section.*

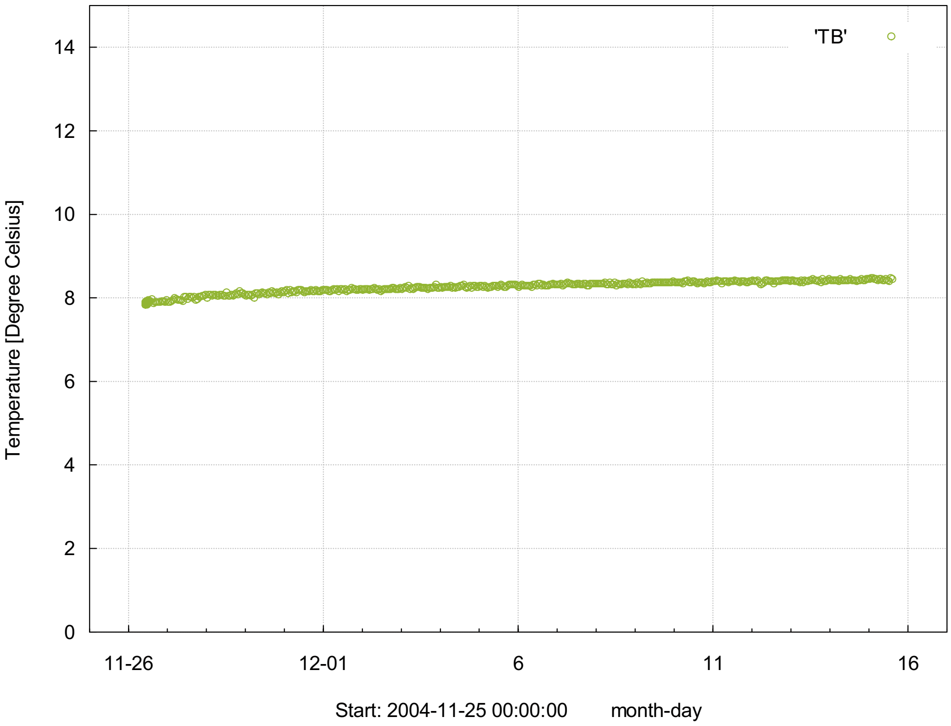


Figure A5-5. *Temperature of the groundwater in the borehole section (TB).*

Appendix 6

Chemmac measurements (Eh, pH, electrical conductivity, dissolved oxygen and temperature) section 408.0–415.3 m

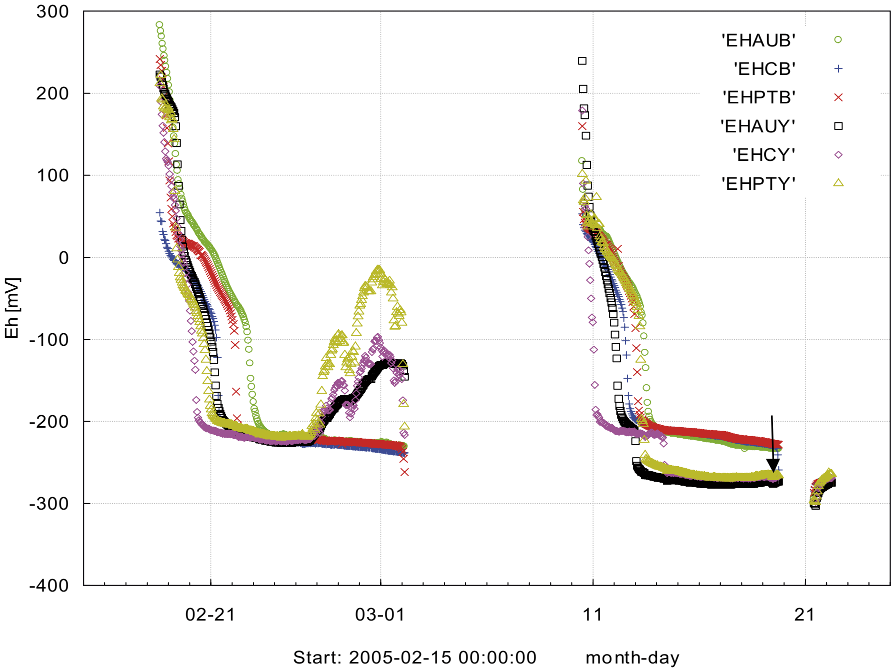


Figure A6-1. Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.

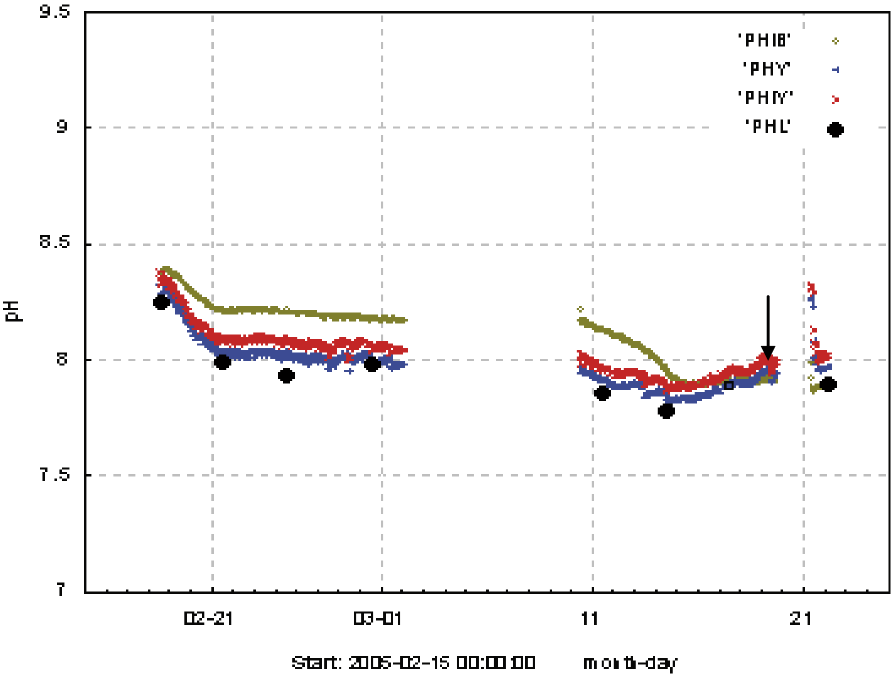


Figure A6-2. Measurements of pH by one glass electrode in the borehole section (PHIB) and two glass electrodes at the surface (PHY and PHIY). The response from PHB was not stable and was therefore rejected. The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.

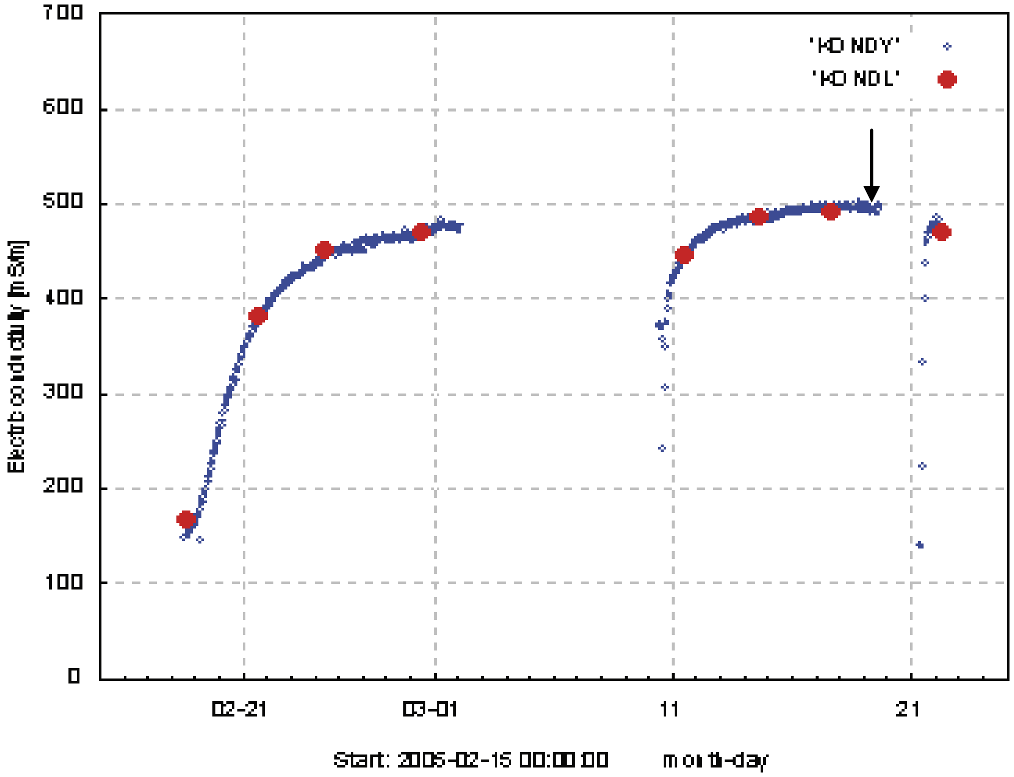


__Figure A6-3.__ Electrical conductivity measurement in the surface measurement cell (KONDY). The laboratory conductivity in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.

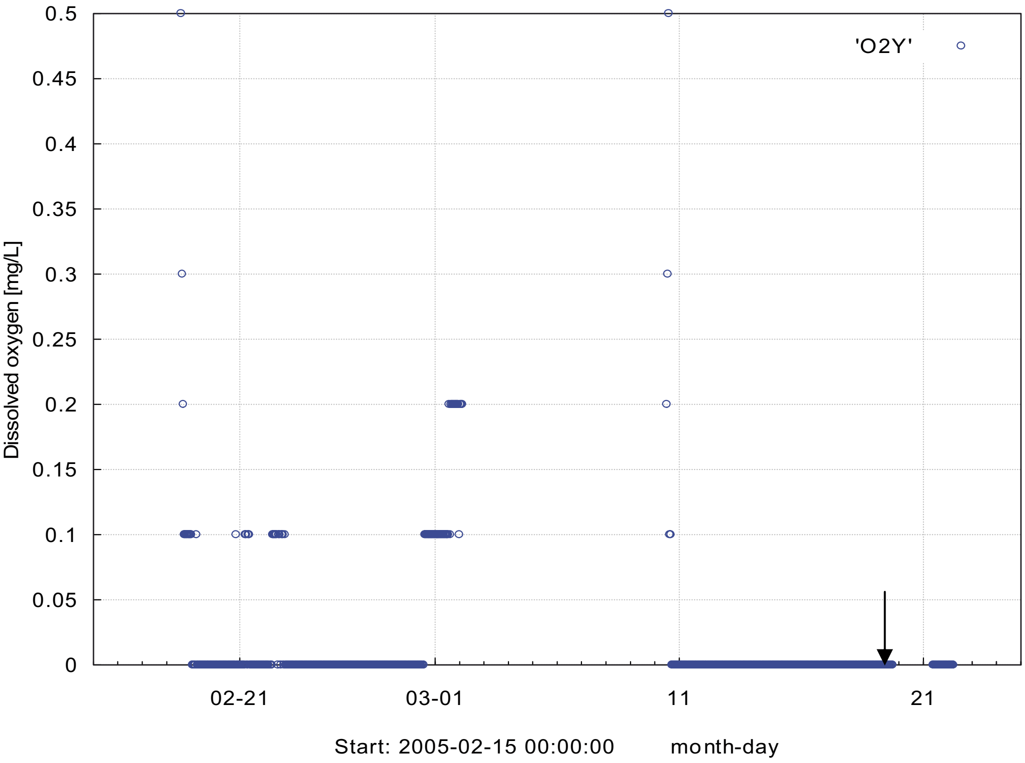


__Figure A6-4.__ Dissolved oxygen measurement (O2Y) in the surface measurement cell. The arrow shows the chosen representative value for dissolved oxygen in the borehole section.

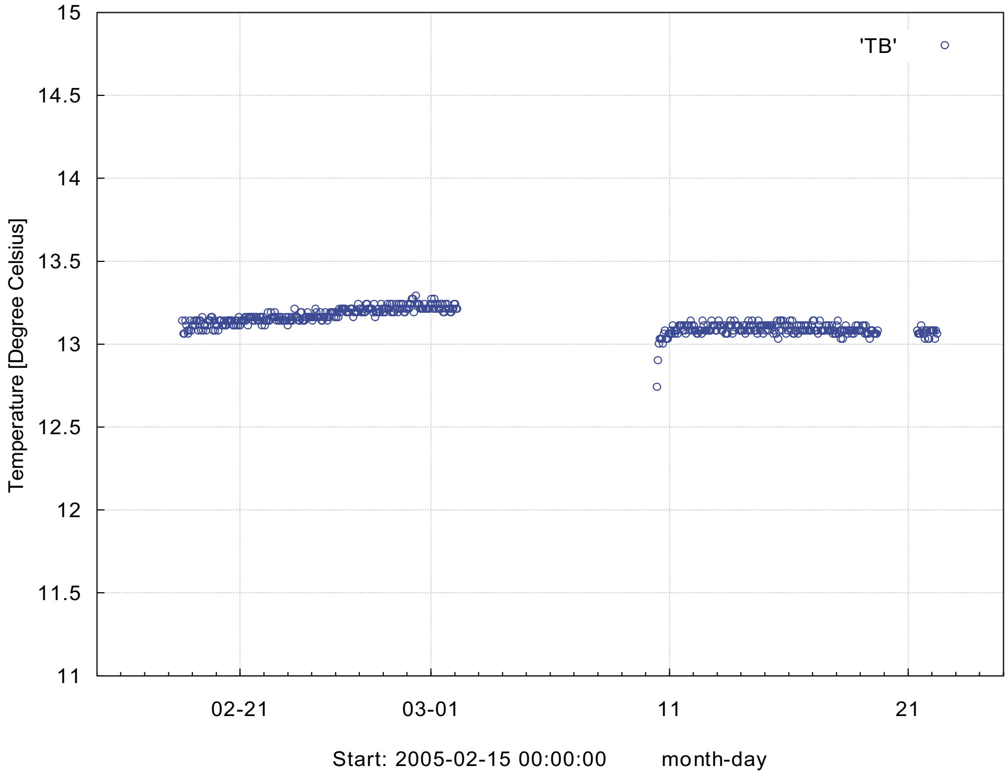


Figure A6-5. *Temperature of the groundwater in the borehole section (TB).*

Appendix 7

Chemmac measurements (Eh, pH, electrical conductivity, dissolved oxygen and temperature) section 735.5–748.0 m

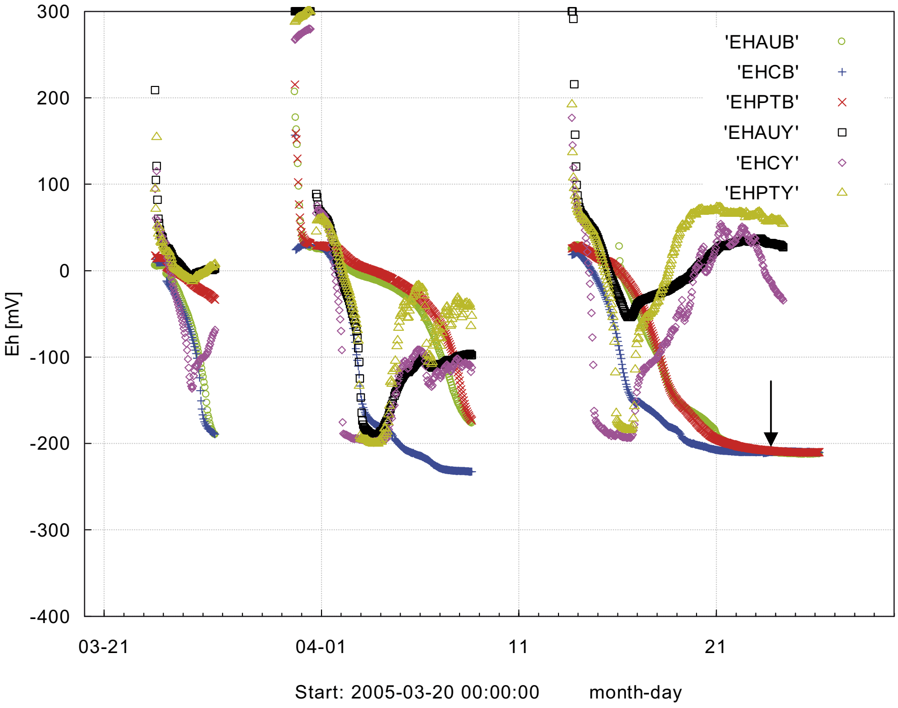


Figure A7-1. *Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.*

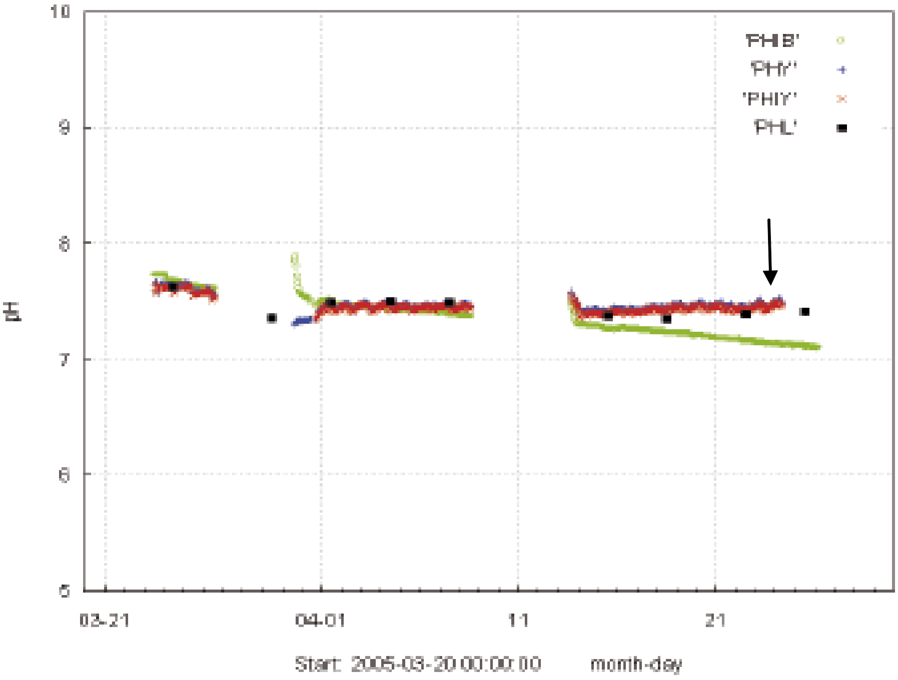


Figure A7-2. *Measurements of pH by one glass electrodes in the borehole section (PHIB) and two glass electrodes at the surface (PHY and PHIY). The response from PHB was not stable and was therefore rejected. The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.*

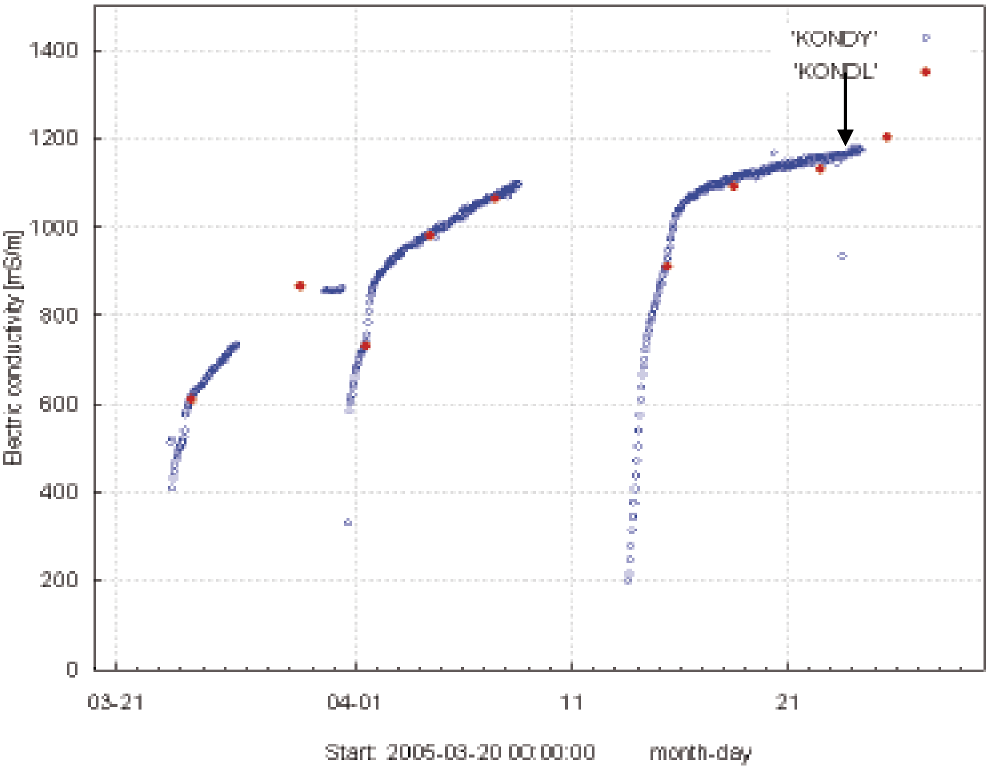


Figure A7-3. *Electrical conductivity measurement in the surface measurement cell (KONDY). The laboratory conductivity in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.*

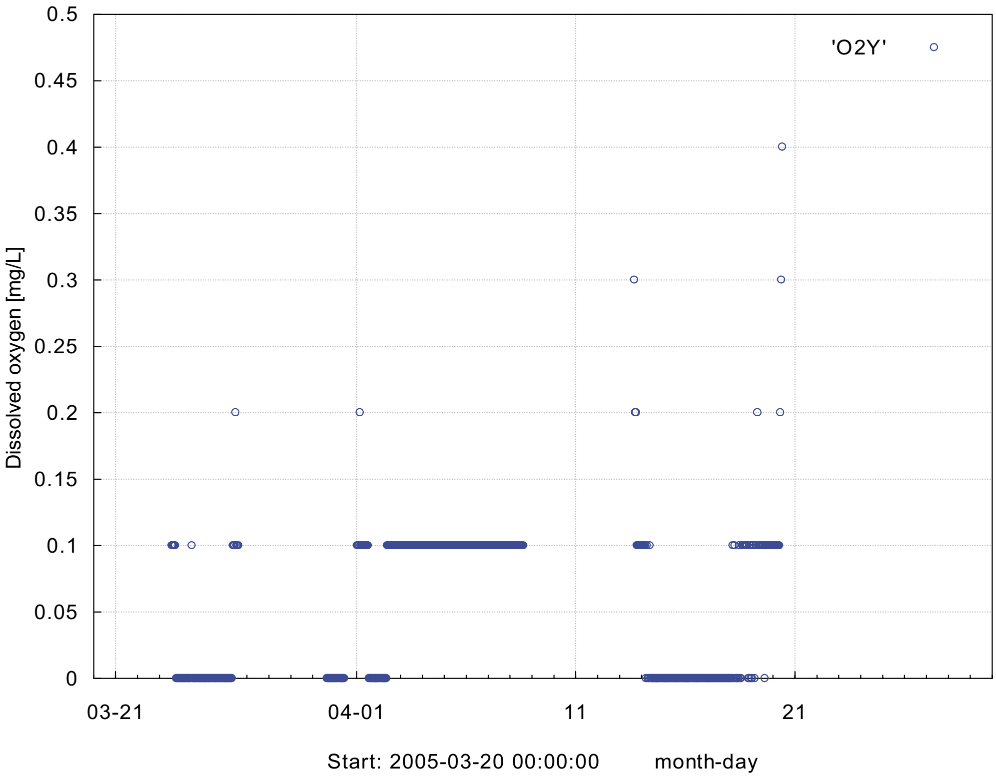


Figure A7-4. *Dissolved oxygen measurement (O2Y) in the surface measurement cell.*

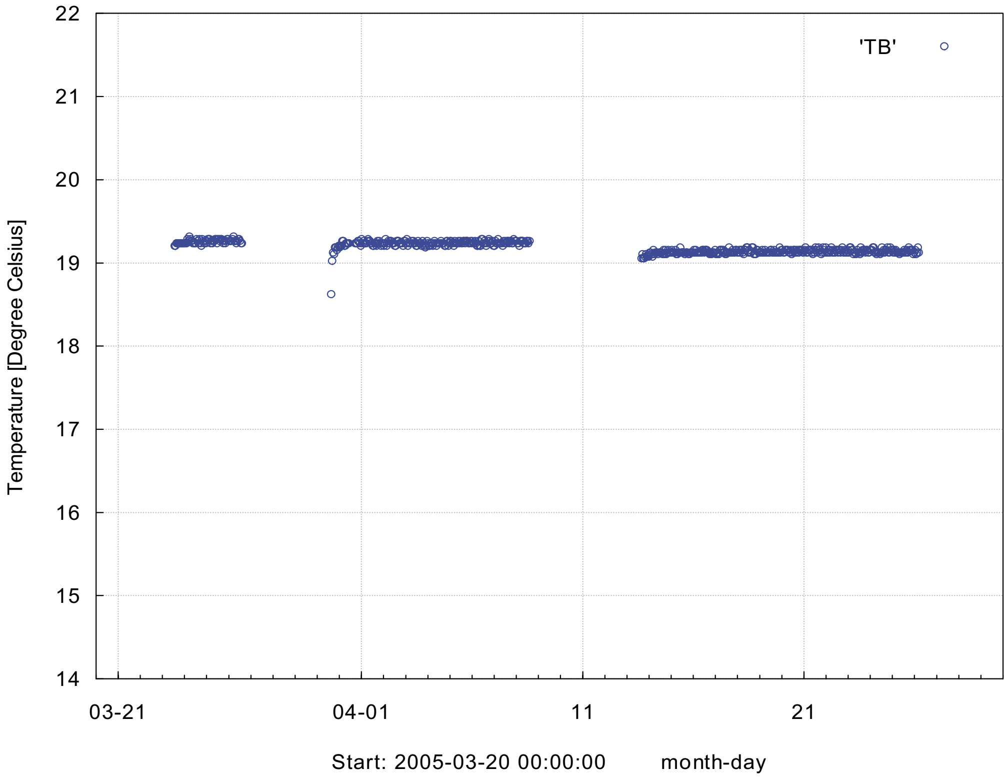


Figure A7-5. *Temperature of the groundwater in the borehole section (TB).*

Appendix 8

Chemmac measurements (Eh, pH, electrical conductivity, dissolved oxygen and temperature) section 964.5–975.2 m

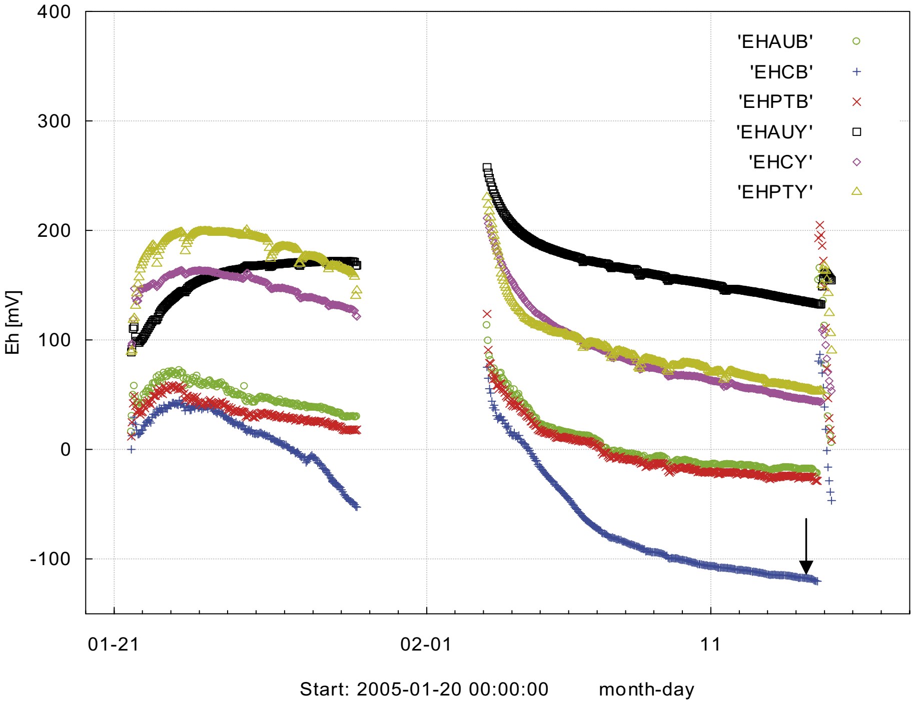


***Figure A8-1.** Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh value for the borehole section.*

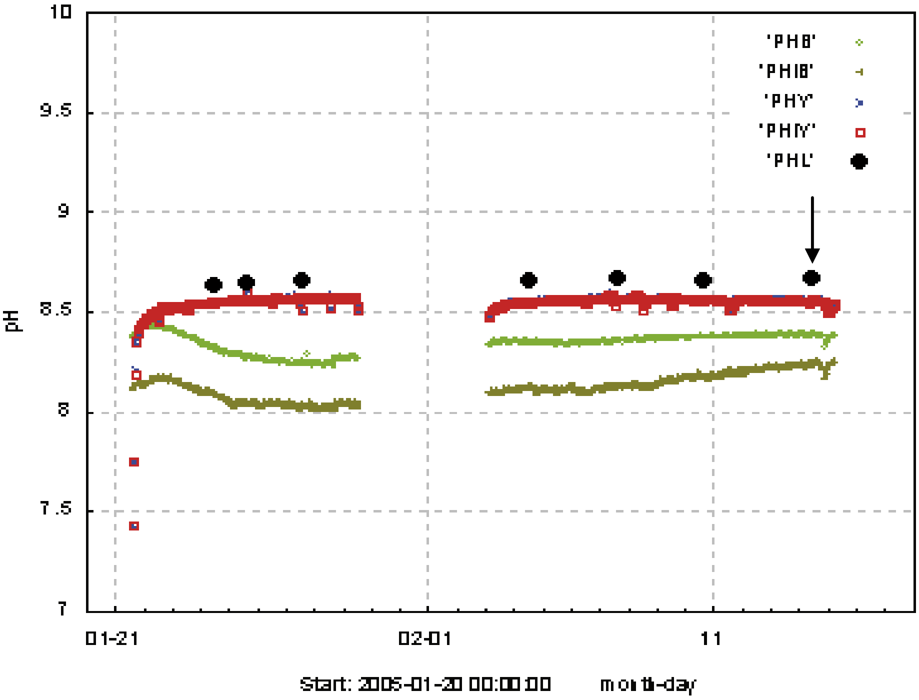


***Figure A8-2.** Measurements of pH by two glass electrodes in the borehole section (PHB and PHIB) and two glass electrodes at the surface (PHY and PHIY). The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.*

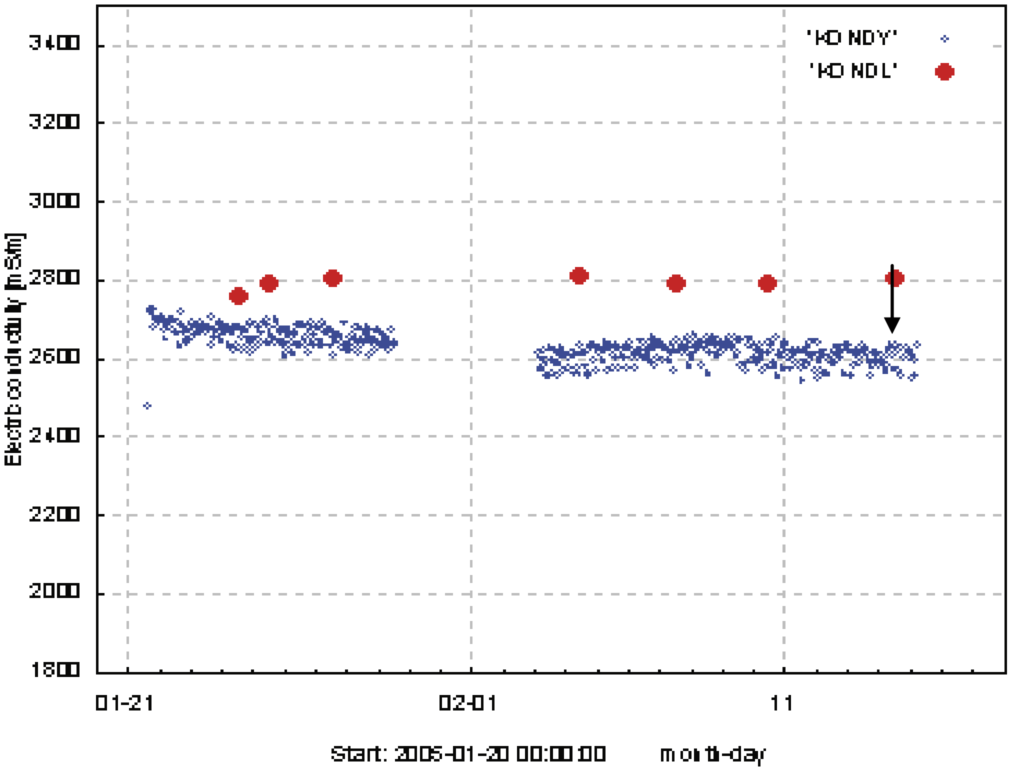


Figure A8-3. *Electrical conductivity measurement in the surface measurement cell (KONDY). The laboratory conductivity measured in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.*

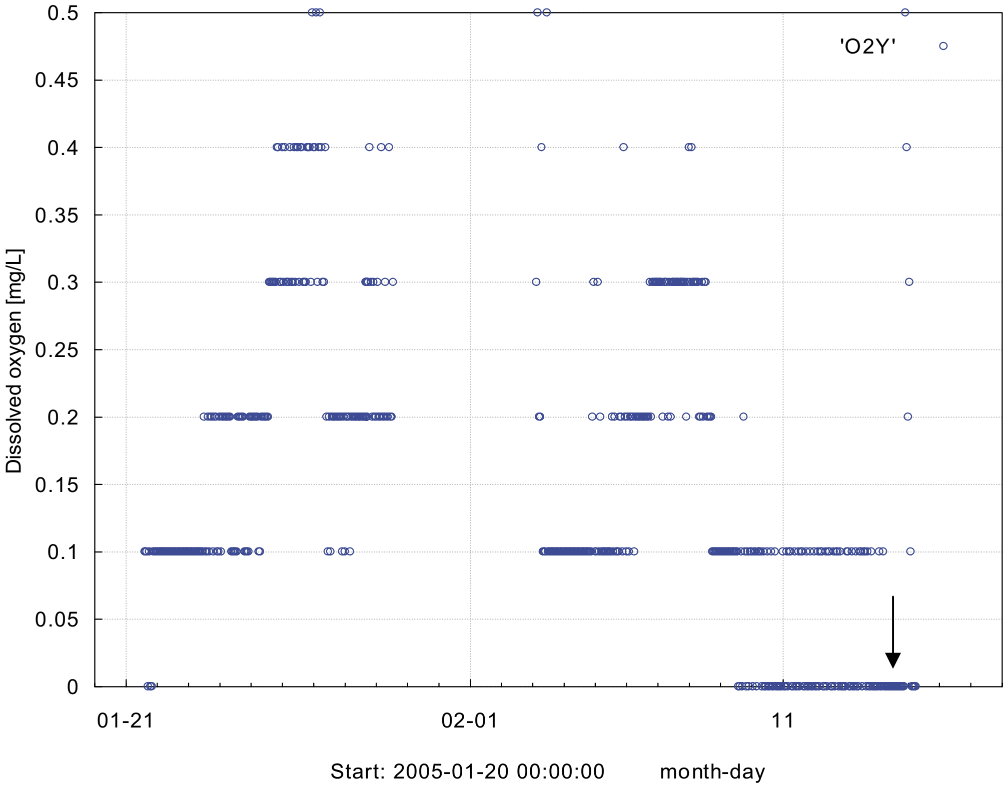


Figure A8-4. *Dissolved oxygen measurement (O2Y) in the surface measurement cell. The arrow shows the chosen representative value for dissolved oxygen in the borehole section.*

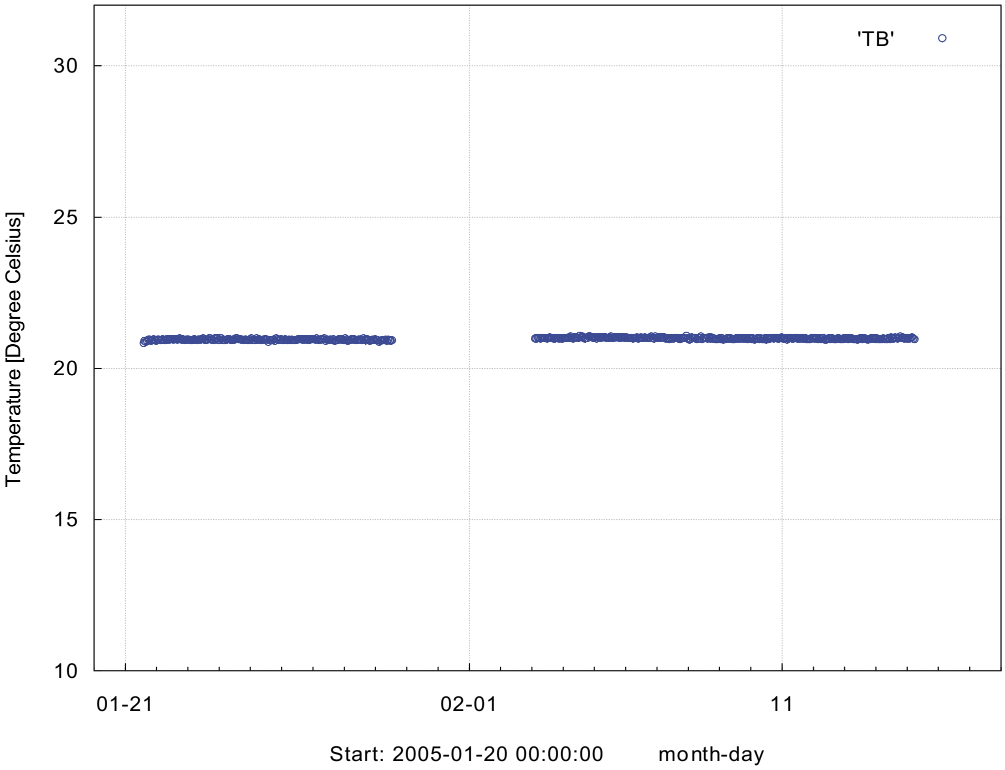


Figure A8-5. *Temperature of the groundwater in the borehole section (TB).*

Appendix 9

Sampling and analysis methods

Table A9-1. Sample handling routines and analysis methods.

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Laboratory***	Analysis within – or delivery time to lab.	Included in SKB class
Drill water	Uranine	Glass (brown)	100	No	No	Spectrofluorometry	Äspö chemistry lab.	–	2,4,5
Anions	HCO_3 pH(lab) cond (lab)	Plastic	250	No	No	Titration Pot. meas, Cond. meas.	Äspö chemistry lab.	The same day – maximum 24 hours	2,4,5
	SO_4, Br^-, F^-, Cl^-	Plastic	250	Yes (in connection with analysis)	No	Titration (Cl^-) IC (Cl^-, SO_4, Br^-, F^-) ISE (F^-)	Äspö chemistry lab.	Not critical (month)	4,5
	Br^-	Plastic	100	Yes	No	ICP MS	Analytica AB (Control laboratory for Br^-)	Not critical (month)	5
	I^-	Plastic	100	Yes	No	ICP MS	Analytica AB	Not critical (month)	4,5
Cations, Si and S	Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr	Plastic (acid washed)	100	Yes	Yes (1 mL HNO_3)	ICP AES ICP MS	Analytica AB, (Control laboratory AnalyCen)	Not critical (month)	4,5
Cations	Fe, Mn	Plastic (acid washed)	100	Yes	Yes (1mL HNO_3)	ICP AES ICP MS	Analytica AB, (Control laboratory AnalyCen)	Not critical (month)	4,5
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic-PEH (acid washed)	500	Yes	Yes (5 mL HCl)	Spectrophotometry Ferrozine method	Äspö chemistry lab.	As soon as possible the same day	4,5
Hydrogen sulphide	HS^-	Glass (Winkler)	About 120×2	Yes	Ev 1 mL 1 M NaOH+ 1 mL 1M ZnAc	Spectrophotometry	Äspö chemistry lab.	Immediately or if conserved, a few days	4,5
Nutrient salts	NO_2, NO_3+NO_2, PO_4	Plastic	250	Yes	No Frozen	Spectrophotometry	Dept. of System ecology		4,5
	NH_4	Glass flask	50	No	No	Spectrophotometry	Äspö chemistry lab.	Maximum 24 hours	4,5
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	Analytica AB	Not critical (month)	5

Component group	**Component/ element**	**Sample container (material)**	**Volume (mL)**	**Filtering**	**Preparation/ Conservation***	**Analysis method**	**Laboratory*** **	**Analysis within – or delivery time to lab.**	**Included in SKB class**
Metal	In	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP AES ICP MS	Analytica AB	Not critical (month)	5
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	Analytica AB	Not critical (month)	5
Dissolved organic Carbon	DOC	Plastic	250	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Paavo Ristola OY	Short transportation time	4,5
Total organic Carbon	TOC	Plastic	250	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Paavo Ristola OY	Short transportation time	5
Environmental isotopes	$\partial^{2}H$, $\partial^{18}O$	Plastic	100	No	– –	MS	IFE	Not critical (month)	2,4,5
Tritium,	^{3}H (enhanced.)	Plastic (dry bottle)	500	No	–	LSC	Univ. of Waterloo	Not critical (month)	2,4,5
Chlorine-37	$\partial^{37}Cl$	Plastic	100	No	–	ICP MS	Univ. of Waterloo	Not critical (month)	5
Carbon isotopes	$\partial^{13}C$, pmC (^{14}C)	Glass (brown)	100×2	No	–	(A)MS	Univ. of Waterloo	A few days	5
Sulphur isotopes	$\partial^{34}S$	Plastic	1,000	No	–	Combustion, ICP MS	IFE	No limit	5
Strontium-isotopes	$^{87}Sr/^{86}Sr$	Plastic	100	No	–	TIMS	IFE	Days or Week	5
Uranium and Thorium isotopes	^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th,	Plastic	100	No	–	Chemical separat. Alfa/gamma spectrometry	IFE	No limit	5
Boron isotopes	$^{10}B/^{11}B$	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP MS	Analytica AB	No limit	5
Radon and Radium isotopes	^{222}Rn, ^{226}Ra	Plastic	500	No	No	EDA, RD-200	IFE	Immediate transport	5
Dissolved gas (content and composition)	Ar, N_2, CO_2, O_2, CH_4, H_2, CO, C_2H_2, C_2H_4, C_2H_6, C_3H_8	Cylinder of stainless steel	200	No	No	GC	Paavo Ristola OY	Immediate transport	5
Colloids	Filter series and fractionation (see below)	Polycarbonate filter	0.45, 0.2 and 0.05 µm	–	N_2 atmosphere	ICP AES ICP MS	Analytica AB	Immediate transport	5

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Laboratory***	Analysis within – or delivery time to lab.	Included in SKB class
Humic and fulvic acids, fractionation	DOC	Fractions are collected in plastic bottles	250	–	N_2 atmosphere	UV oxidation, IR	Paavo Ristola OY	Immediate transport	5
Humic and fulvic acids, fractionation	1) Environmental metals 2) Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr, Fe and Mn	1) Plastic 2) Plastic (acid washed bottles)	1) 100 2) 100	1) Yes 2) Yes	1) Yes (1 mL HNO_3) 2) Yes (1 mL HNO_3)	1) ICP AES ICP MS 2) ICP AES ICP MS	1) Analytica AB 2) Analytica AB	Not critical (month)	5
Carbon isotopes in humic and fulvic acids	∂^{13}C, pmC (^{14}C)	DEAE cellulose (anion exchanger)	–	–	–	(A)MS	The Ångström laboratory, Uppsala	A few days	5
Density	Density	Plast	250	No	–	Pycnometer	Äspö chemistry lab.	–	Last SKB class 5 sample in each section.
Archive samples with acid	–	Plast (washed in acid)	100×2**	Yes	Yes (1 mL HNO_3)	–	–	Storage in freeze container	4,5
Archive samples without acid	–	Plastic	250×2**	Yes	No	–	–	Storage in freeze container	2,4,5

* Suprapur acid is used for conservation of samples.

** Minimum number, the number of archive samples can vary depending on how many similar samples that are collected at the same occasion.

*** Full name and address is given in Table A2-3.

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
LSC	Liquid Scintillation Counting
(A)MS	(Accelerator) Mass Spectrometry
GC	Gas Chromatography

Table A9-2. Reporting limits and measurement uncertainties.

Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainty[2]	”Total” uncertainty[3]
Uranine	Spectro-fluorometry	0.05		µg/L	15%	15%
pH	Pot. meas.	–	–	–	5%	–
Cond.	Cond. meas.	0.02	1	mS/m	4%	–
HCO^-_3	Alkalinity titration	0.2	1	mg/L	4%	< 10%
Cl^-	Mohr titration	5	70	mg/L	5%	< 10%
Cl^-	IC	0.2	0.5		6%	10%
SO_4	IC	0.2	0.5	mg/L	6%	15%
Br^-	IC	0.2	0.7	mg/L	9%	20%
Br^-	ICP	–	0.001–0.010[1]		15%	
F^-	IC	0.2	0.6	mg/L	10%	20%
F^-	Potentiometri	–	–		–	–
I^-	ICP	–	0.001–0.010[1]	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	10%	15%
Si(tot)	ICP	–	0.03	mg/L	4%	15%
Sr	ICP	–	0.002	mg/L	4%	15%
Li	ICP	–	0.2–2[1]	µg/L	10%	20%
Fe	ICP	–	0.4–4[1]	µg/L	6%	10%
Mn	ICP	–	0.03–0.1	µg/L	8%	10%
Al, Zn	ICP	–	0.2–0.7[1]	µg/L	12%	–
Ba, Cr, Mo, Pb	ICP	–	0.01–0.3[1]	µg/L	7–10%	–
Cd, Hg	ICP	–	0.002–0.5[1]	µg/L	9 and 5% resp.	–
Co, V	ICP	–	0.005–0.05[1]	µg/L	8 and 5% resp.	–
Cu	ICP	–	0.1–0.5[1]	µg/L	8%	–
Ni	ICP	–	0.05–0.5[1]	µg/L	8%	–
P	ICP	–	1–40[1]	µg/L	6%	15%
As	ICP	–	0.01–0.5[1]	µg/L	20%	Within the same size (low conc.)
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Y, Hf	ICP	–	0.005–0.05[1]	µg/L	10%	Within the same size (low conc.)
Sc, In, Th	ICP	–	0.05–0.5[1]	µg/L	10%	Within the same size (low conc.)
Rb, Zr, Sb, Cs, Tl	ICP	–	0.025–0.25[1]	µg/L	10%	Within the same size (low conc.)
U	ICP	–	0.001–0.01[1]	µg/L	12%	Within the same size (low conc.)
Fe(II), Fe(tot)	Spectro-photometry	5	20	µg/L	15% (>30 µg/L)	20%

Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainty[2]	"Total" uncertainty[3]
NH_4-N	Spectro-photometry	3	11–50 > 50	µg/L	10 µg/L 23%	–
PO_4-P	Spectro-photometry	–	0.5–20 > 20	µg/L	0.4 µg/L 2.2%	15%
NO_2-N	Spectro-photometry	–	0.1–20 > 20	µg/L	0.1 µg/L 2%	15%
NO_2-N + NO_3-N	Spectro-photometry	–	0.2–20 > 20	µg/L	0.2 µg/L 2.5%	15%
HS^-	Spectro-photometry	2	30–200 200–500	µg/L	30 µg/L 18%	20%
DOC	See Table A9-1	–	0.5	mg/L	8%	30%
TOC	See Table A9-1	–	0.5	mg/L	10%	30%
$\delta^{2}H$	MS	–	2	‰ SMOW[4]	1.0‰	–
$\delta^{18}O$	MS	–	0.1	‰ SMOW[4]	0.2‰	–
^{3}H	LSC	–	0.8 or 0.1	TU[5]	0.8 or 0.1 TU	–
$\delta^{37}Cl$	ICP MS	–	0.2‰ (20 mg/L)	‰ SMOC[6]	–	–
$\delta^{13}C$	A (MS)	–	> 20 mg carbon	‰ PDB[7]	–	–
pmC (^{14}C)	A (MS)	–	> 20 mg carbon	PmC[8]	–	–
δ^{34} S	ICP MS	–	0.2‰	‰ CDT[9]	0.2‰	–
$^{87}Sr/^{86}Sr$	MS	–	–	No unit (ratio)[10]	0.000020	–
$^{10}B/^{11}B$	ICP MS	–	–	No unit (ratio)[10]	0.0020	–
^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th	Alfa spectr.	–	0.05	Bq/L[11]	0.05 Bq/L	Right order of magnitude
^{222}Rn, ^{226}Rn	LSC	–	0.1	Bq/L	0.05 Bq/L	
Density	Pycnometer			g/mL	0.15%	Within the same size

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. Per mill deviation[11] from SMOW (Standard Mean Oceanic Water).
5. TU = Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of 10^{-18} (1 Bq/L Tritium = 8.45 TU).
6. Per mill deviation[11] from SMOC (Standard Mean Oceanic Chloride).
7. Per mill deviation[11] from PDB (the standard PeeDee Belemnite).
8. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age:
   $pmC = 100 \times e^{((1950-y-1.03t)/8274)}$
   where y = the year of the C-14 measurement and t = C-14 age
9. Per mill deviation[12] from CDT (the standard Canyon Diablo Troilite).
10. Isotope ratio without unit.
11. The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232:
    1 ppm U = 12.4 Bq/kg^{238}U
    1 ppm Th = 3.93 Bq/kg^{232}Th
12. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:
    $\delta^{y}I = 1{,}000 \times (K_{sample} - K_{standard})/K_{standard}$, where K= the isotope ratio and $^{y}I = {}^{2}H$, ^{18}O, ^{37}Cl, ^{13}C or ^{34}S etc.

Table A9-3. Participant laboratories.

Äspö water chemical laboratory (SKB)
Inainööritoimisto Paavo Ristola Oy Teollisuus-ja Voimalaitoskemia Rajantorpantie 8, C-talo 01600 Vantaa FINLAND
Dept. of System ecology Stockholm University 10691 Stockholm
Analytica AB Aurorum 10 977 75 Luleå (Nytorpsvägen 16 Box 511 183 25 Täby)
Environmental Isotope Laboratory Dep. of Earth Sciences University of Waterloo Waterloo, Ontario N2L 3G1 CANADA
Institutt for energiteknik (IFE) Insituttveien 18 P.O Box 40 2027 Kjeller NORGE
AnalyCen Nordic AB Box 905 531 19 Lidköping
The Ångström laboratory Box 534 Se-751 21 Uppsala

Compilation of water analysis data

Table A10-1. Water composition. Compilation November 2005.

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	FeII mg/L
KLX03A	193.50	198.37	7946	2004-11-26		–	–	–	–	323	297	–	–	–	–	–	–	–	–
KLX03A	193.50	198.37	7947	2004-11-29	0.08	274	2.96	36.4	5.4	328	279	37.2	13.2	xx	3.22	6.10	0.209	0.187	0.175
KLX03A	193.50	198.37	7948	2004-12-01	–0.03	270	2.97	35.4	5.3	332	270	36.8	13.1	xx	2.96	6.10	0.218	0.216	0.205
KLX03A	193.50	198.37	7949	2004-12-03	0.18	267	2.93	34.8	5.2	327	265	36.5	13.0	xx	3.07	6.10	0.259	0.247	0.232
KLX03A	193.50	198.37	7950	2004-12-06	0.04	266	2.9	34.4	5.2	331	262	36.4	12.9	xx	3.13	6.20	0.320	0.304	0.294
KLX03A	193.50	198.37	7951	2004-12-09	–1.23	260	2.91	33.3	5.0	335	260	36.5	13.0	xx	3.12	5.90	0.359	0.324	0.307
KLX03A	193.50	198.37	7952	2004-12-13	–1.49	259	2.85	32.7	5.0	335	260	36.4	12.7	xx	3.18	5.90	0.294	0.284	0.254
KLX03A	193.50	198.37	7953	2004-12-15	–1.76	255	2.84	32	4.9	328	259	36.6	12.6	xx	3.21	5.80	0.264	0.266	0.251
KLX03A	193.50	198.37	7954	2004-12-15		–	–	–	–	332	259	36.6	–	0.966	3.19	–	–	0.257	0.249
KLX03A	408.00	415.30	10082	2005-02-18		–	–	–	–	316	344	–	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10083	2005-02-21	1.78	631	5.21	167	8.9	223	1,040	96.8	35.5	xx	2.95	6.82	0.876	1.00	0.971
KLX03A	408.00	415.30	10084	2005-02-23		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10085	2005-02-24	1.24	732	5.86	214	10.4	204	1,290	116	41.6	xx	2.35	6.61	1.03	1.13	1.11
KLX03A	408.00	415.30	10086	2005-02-28	0.90	759	5.76	225	10.6	196	1,360	122	43.0	xx	2.90	6.34	0.355	0.385	0.371
KLX03A	408.00	415.30	10087	2005-03-10		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10088	2005-03-11	0.75	719	5.68	209	10.1	194	1,280	116	40.8	xx	3.05	6.73	0.814	0.816	0.816
KLX03A	408.00	415.30	10089	2005-03-14	0.86	780	5.75	232	10.8	178	1,410	126	45.0	xx	3.80	6.64	0.779	0.783	0.791
KLX03A	408.00	415.30	10090	2005-03-17	1.36	797	5.52	241	11.0	185	1,430	129	46.2	xx	3.00	6.49	0.682	0.732	0.717
KLX03A	408.00	415.30	10091	2005-03-22	1.92	791	5.51	234	10.8	189	1,390	127	45.3	xx	2.90	6.51	0.408	0.435	0.429
KLX03A	408.00	415.30	10183	2005-03-22		–	–	–	–	188	1,150	105	–	7.17	2.90	–	–	0.429	0.422
KLX03A	660.00	670.65	10002	2005-01-19		–	–	–	–	25	4,010	405	–	xx	1.15	–	–	–	–
KLX03A	660.00	670.65	10003	2005-01-20		–	–	–	–	–	–	–	–	–	–	–	–	–	–

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	FeII mg/L
KLX03A	660.00	670.65	10004	2005-01-21		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10184	2005-03-23		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10185	2005-03-24		–	–	–	–	163	1,840	185	–	xx	2.07	–	–	–	–
KLX03A	735.50	748.04	10186	2005-03-29		–	–	–	–	85.2	2,780	278	–	xx	1.76	–	–	2.14	2.09
KLX03A	735.50	748.04	10187	2005-03-31		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10188	2005-04-01	0.94	969	9.81	579	11.2	113	2,250	232	85.9	xx	3.80	7.56	1.71	1.85	1.90
KLX03A	735.50	748.04	10189	2005-04-04	–2.42	1,130	9.82	861	11.8	65.5	3,180	311	115	xx	0.80	8.02	0.839	1.15	1.15
KLX03A	735.50	748.04	10190	2005-04-05		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10191	2005-04-07	–0.24	1,300	11.4	974	12.6	52.4	3,480	337	127	xx	0.90	7.19	0.896	1.04	1.03
KLX03A	735.50	748.04	10192	2005-04-08		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10193	2005-04-14		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10194	2005-04-15	–1.83	1,130	10.9	784	12.9	76.4	3,010	305	108	xx	1.96	7.37	1.8	2.14	2.15
KLX03A	735.50	748.04	10239	2005-04-18	–0.15	1,320	11.6	1,050	13.2	45.1	3,630	373	133	xx	1.77	7.04	1.12	1.26	1.25
KLX03A	735.50	748.04	10240	2005-04-19		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10241	2005-04-22	–2.73	1,380	11.1	993	12.9	38.0	3,820	391	140	xx	1.59	8.02	1.09	1.14	1.13
KLX03A	735.50	748.04	10242	2005-04-25	–0.87	1,450	10.9	1,090	12.8	33.5	3,940	398	146	xx	1.78	8.00	0.872	0.917	0.903
KLX03A	735.50	748.04	10243	2005-04-25		–	–	–	–	33.6	3,950	407	–	37.2	1.78	–	–	0.934	0.859
KLX03A	964.50	975.15	10005	2005-01-24		–	–	–	–	7	10,600	–	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10006	2005-01-25	1.08	2,860	8.52	3,800	2.1	8	10,400	742	230	xx	<0.2	5.20	<0.100	0.077	0.068
KLX03A	964.50	975.15	10007	2005-01-27	0.59	2,860	8.58	3,730	2.1	7	10,400	741	221	xx	<0.2	5.20	<0.004	<0.005	<0.005
KLX03A	964.50	975.15	10008	2005-02-03		–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10009	2005-02-04	0.49	2,850	8.65	3,730	2.1	8	10,400	751	226	xx	<0.2	5.20	<0.004	<0.005	<0.005
KLX03A	964.50	975.15	10074	2005-02-07	0.67	2,860	8.46	3,750	2.1	7.39	10,400	752	229	xx	<0.2	5.21	<0.100	<0.005	<0.005
KLX03A	964.50	975.15	10075	2005-02-10	–14.15	2,090	5.94	2,800	1.6	7.74	10,500	749	172	xx	<0.2	3.90	<0.100	<0.005	<0.005
KLX03A	964.50	975.15	10076	2005-02-14	0.63	2,880	8.57	3,780	2.1	7.7	10,500	758	226	xx	<0.2	5.22	<0.004	<0.005	<0.005
KLX03A	964.50	975.15	10077	2005-02-14		–	–	–	–	7.95	10,400	749	–	109	<0.2	–	–	0.013	<0.005

Table A10-1. Continue.

Idcode	Secup m	Seclow m	Sample no.	Mn mg/L	Li mg/L	Sr mg/L	I^- mg/L	pH	DOC mg/L	TOC mg/L	HS^- mg/L	Drill_water %	ElCond mS/m	NH_4N mg/L	NO_2N mg/L	NO_3N mg/L	NO_2N/NO_3N mg/L	PO_4P mg/L	Density g/mL
KLX03A	193.50	198.37	7946	–	–	–	–	8.19	–	–	–	0.25	152	–	–	–	–	–	–
KLX03A	193.50	198.37	7947	0.07	0.032	0.67	0.025	8.20	19	–	<0.002	0.24	143	0.0573	0.0001	0.0010	0.0011	0.0036	–
KLX03A	193.50	198.37	7948	0.06	0.032	0.65	0.025	8.19	20	20	0.002	0.25	141	0.0593	0.0001	<0.0002	0.0002	0.0030	–
KLX03A	193.50	198.37	7949	0.06	0.031	0.64	0.024	8.20	19	–	<0.002	0.26	143	0.0534	0.0001	<0.0002	0.0002	0.0030	–
KLX03A	193.50	198.37	7950	0.06	0.031	0.63	0.025	8.21	19	20	<0.002	0.25	143	0.0467	0.0002	<0.0002	0.0002	0.0029	–
KLX03A	193.50	198.37	7951	0.07	0.032	0.61	0.028	8.19	22	–	<0.002	0.29	141	0.0533	0.0001	0.0002	0.0002	0.0024	–
KLX03A	193.50	198.37	7952	0.06	0.029	0.61	0.029	8.21	21	20	0.004	0.24	141	0.0449	0.0001	<0.0002	0.0002	0.0024	–
KLX03A	193.50	198.37	7953	0.06	0.029	0.60	0.027	8.20	21	20	<0.002	0.24	142	0.0590	0.0001	0.0002	0.0003	0.0024	0.9971
KLX03A	193.50	198.37	7954	–	–	–	–	8.22	–	–	0.002	0.24	141	0.059	–	–	–	–	–
KLX03A	408.00	415.30	10082	–	–	–	–	8.25	–	–	–	0.85	165	–	–	–	–	–	–
KLX03A	408.00	415.30	10083	0.114	0.073	3.40	0.078	7.99	15	–	0.013	3.30	380	0.0275	0.0001	<0.0002	<0.0002	0.0022	–
KLX03A	408.00	415.30	10084	–	–	–	–	–	–	–	–	3.02	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10085	0.115	0.083	4.44	0.069	7.94	13	14	0.008	2.84	448	0.0360	0.0001	<0.0002	<0.0002	0.0035	–
KLX03A	408.00	415.30	10086	0.106	0.085	4.69	0.084	7.98	13	–	0.004	2.31	469	0.0389	<0.0001	<0.0002	<0.0002	0.0031	–
KLX03A	408.00	415.30	10087	–	–	–	–	–	–	–	–	0.72	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10088	0.126	0.082	4.28	0.080	7.86	16	–	0.005	1.71	446	0.0292	0.0002	0.0002	0.0005	0.0020	–
KLX03A	408.00	415.30	10089	0.131	0.089	4.78	0.087	7.79	17	–	0.004	2.06	487	0.0172	0.0001	0.0005	0.0006	0.0013	–
KLX03A	408.00	415.30	10090	0.116	0.089	4.92	0.073	7.89	13	12	0.004	1.95	492	0.0275	0.0002	0.0002	0.0004	0.0022	–
KLX03A	408.00	415.30	10091	0.107	0.087	4.84	0.071	7.89	13	12	0.009	1.88	469	0.0337	0.0001	<0.0002	0.0002	0.0025	0.9982
KLX03A	408.00	415.30	10183	–	–	–	–	7.89	–	–	0.009	1.90	470	0.0355	–	–	–	–	–
KLX03A	660.00	670.65	10002	–	–	–	–	7.53	–	–	–	9.67	1,200	–	–	–	–	–	–
KLX03A	660.00	670.65	10003	–	–	–	–	–	–	–	–	12.70	–	–	–	–	–	–	–
KLX03A	660.00	670.65	10004	–	–	–	–	–	–	–	–	12.80	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10184	–	–	–	–	–	–	–	–	2.79	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10185	–	–	–	–	7.63	–	–	–	3.97	606	–	–	–	–	–	–
KLX03A	735.50	748.04	10186	–	–	–	–	7.36	–	–	0.003	8.04	866	0.0289	–	–	–	–	–
KLX03A	735.50	748.04	10187	–	–	–	–	–	–	–	–	3.13	–	–	–	–	–	–	–

Idcode	Secup m	Seclow m	Sample no.	Mn mg/L	Li mg/L	Sr mg/L	I^- mg/L	pH	DOC mg/L	TOC mg/L	HS^- mg/L	Drill_water %	ElCond mS/m	NH_4N mg/L	NO_2N mg/L	NO_3N mg/L	NO_2N/NO_3N mg/L	PO_4P mg/L	Density g/mL
KLX03A	735.50	748.04	10188	0.270	0.151	10.8	0.126	7.49	9.8	–	0.007	6.83	731	0.0189	0.0001	<0.0002	0.0002	<0.0005	–
KLX03A	735.50	748.04	10189	0.287	0.209	16.8	0.166	7.50	7.0	–	<0.002	8.66	982	xx	0.0001	0.0005	0.0006	<0.0005	–
KLX03A	735.50	748.04	10190	–	–	–	–	–	–	–	–	9.51	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10191	0.257	0.220	18.9	0.185	7.49	5.7	–	0.003	9.67	1,060	0.0213	0.0001	<0.0002	0.0002	<0.0005	–
KLX03A	735.50	748.04	10192	–	–	–	–	–	–	–	–	9.75	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10193	–	–	–	–	–	–	–	–	8.57	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10194	0.325	0.184	15.0	0.153	7.38	8.0	8.1	0.008	10.2	909	0.0116	0.0001	<0.0002	0.0002	<0.0005	–
KLX03A	735.50	748.04	10239	0.291	0.239	19.6	0.190	7.35	5.1	–	<0.002	10.2	1,090	0.0158	0.0001	<0.0002	0.0002	<0.0005	–
KLX03A	735.50	748.04	10240	–	–	–	–	–	–	–	–	10.5	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10241	0.345	0.232	22.0	0.014	7.39	4.3	4.5	0.005	10.6	1,130	0.0207	0.0003	<0.0002	0.0003	0.0005	–
KLX03A	735.50	748.04	10242	0.29	0.239	23.1	0.046	7.41	4.0	4.0	0.008	10.8	1,200	0.0257	0.0002	<0.0002	0.0002	<0.0005	1.0014
KLX03A	735.50	748.04	10243	–	–	–	–	7.44	–	–	<0.002	11.0	1,190	0.0204	–	–	–	–	–
KLX03A	964.50	975.15	10005	–	–	–	–	8.64	–	–	–	0.15	2,760	–	–	–	–	–	–
KLX03A	964.50	975.15	10006	<0.02	0.448	71.2	0.435	8.65	2.1	–	0.062	0.13	2,790	<0.003	0.0004	0.0002	0.0006	0.0007	–
KLX03A	964.50	975.15	10007	0.02	0.450	71.9	0.428	8.65	2.1	1.5	xx	0.12	2,800	<0.003	0.0001	<0.0002	<0.0002	<0.0005	–
KLX03A	964.50	975.15	10008	–	–	–	–	–	–	–	–	0.09	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10009	0.02	0.445	71.2	0.419	8.66	1.7	1.7	0.067	0.06	2,810	0.0054	0.0001	0.0003	0.0004	0.0005	–
KLX03A	964.50	975.15	10074	<0.02	0.44	71.5	0.446	8.68	1.5	–	0.115	0.05	2,790	<0.003	0.0001	<0.0002	<0.0002	<0.0005	–
KLX03A	964.50	975.15	10075	<0.02	0.327	52.0	0.446	8.65	1.4	1.3	0.105	0.07	2,790	<0.003	0.0002	<0.0002	0.0002	<0.0005	–
KLX03A	964.50	975.15	10076	0.0164	0.467	72.2	0.427	8.68	1.4	1.3	0.115	0.04	2,800	<0.003	0.0001	<0.0002	<0.0002	<0.0005	1.0099
KLX03A	964.50	975.15	10077	–	–	–	–	8.68	–	–	0.135	0.04	2,780	<0.003	–	–	–	–	–

– = Not analysed

A = Results will be reported later

x = No result due to sampling problems

xx = No result due to analytical problems

< “value” = result less than detection limit

ChargeBal % = Rel. charge balance error %

SICADA: water_composition

Table A10-2. Isotopes I (H-, O-, B-, S-, Cl- and C-isotopes). Compilation November 2005.

Idcode	Secup m	Seclow m	Sample no	Sampling date	δ^{2}H dev SMOW	^{3}H TU	δ^{18}O dev SMOW	^{10}B/^{11}B no unit	δ^{34}S dev CDT	δ^{13}C dev PDB	^{87}Sr/^{86}Sr no unit	^{14}C pmC	AGE_BP years	δ^{37}Cl dev SMOC
KLX03A	193.50	198.37	7947	2004-11-29	–81.9	1.5	–11.7	–	–	–	–	–	–	–
KLX03A	193.50	198.37	7948	2004-12-01	–81.3	<0.8	–11.6	0.2302	35.2	–16.89	0.715213	45.18	6,328	–0.54
KLX03A	193.50	198.37	7949	2004-12-03	–80.9	<0.8	–11.5	–	–	–	–	–	–	–
KLX03A	193.50	198.37	7950	2004-12-06	–81.0	<0.8	–11.6	0.2301	36.9	–16.93	0.715252	45.66	6,242	–0.52
KLX03A	193.50	198.37	7951	2004-12-09	–83.1	<0.8	–11.6	–	–	–	–	–	–	–
KLX03A	193.50	198.37	7952	2004-12-13	–85.0	<0.8	–11.5	0.2365	36.3	–16.68	0.715187	45.68	6,239	–0.10
KLX03A	193.50	198.37	7953	2004-12-15	–84.8	<0.8	–11.5	0.2370	37.2	–16.96	0.715229	45.68	6,239	–0.02
KLX03A	193.50	198.37	7954	2004-12-15	–84.8	–	–11.6	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10083	2005-02-21	–97.2	<0.8	–12.5	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10085	2005-02-24	–96.5	<0.8	–12.8	0.2352	15.7	xxx	0.715100	xxx	xxx	xxx
KLX03A	408.00	415.30	10086	2005-02-28	–97.8	<0.8	–12.9	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10088	2005-03-11	–97.1	<0.8	–12.9	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10089	2005-03-14	–97.8	<0.8	–13.2	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10090	2005-03-17	–98.7	<0.8	–13.3	0.2353	14.7	xxx	0.715086	xxx	xxx	0.30
KLX03A	408.00	415.30	10091	2005-03-22	–98.1	xxx	–13.0	0.2354	15.1	xxx	0.715065	xxx	xxx	xxx
KLX03A	408.00	415.30	10183	2005-03-22	–	<0.8	–	–	–	–14.27	–	45.50	6,272	0.40
KLX03A	735.50	748.04	10186	2005-03-29	–	1.6	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10188	2005-04-01	–100.1	<0.8	–12.6	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10189	2005-04-04	–100.4	xxx	–13.0	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10191	2005-04-07	–101.5	1.3	–13.2	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10194	2005-04-15	–100.0	1.0	–12.9	0.2354	11.2	xx	0.715921	xx	xx	0.47
KLX03A	735.50	748.04	10239	2005-03-18	–102.1	<0.8	–13.2	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10241	2005-04-22	–91.7	0.9	–13.6	0.2366	11.8	xx	0.715946	xx	xx	0.55
KLX03A	735.50	748.04	10242	2005-04-25	–92.1	1.2	–13.6	0.2374	11.0	xx	0.715918	xx	xx	0.50
KLX03A	735.50	748.04	10243	2005-04-25	–	–	–	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10006	2004-01-25	–93.4	xx	–12.2	–	–	–	–	–	–	–

Idcode	Secup m	Seclow m	Sample no	Sampling date	δ^{2}H dev SMOW	^{3}H TU	δ^{18}O dev SMOW	^{10}B/^{11}B no unit	δ^{34}S dev CDT	δ^{13}C dev PDB	^{87}Sr/^{86}Sr no unit	^{14}C pmC	AGE_BP years	δ^{37}Cl dev SMOC
KLX03A	964.50	975.15	10007	2005-01-27	–94.8	<0.8	–12.2	0.2420	12.4	xx	0.715771	xx	xx	0.68
KLX03A	964.50	975.15	10009	2005-02-04	–94.9	<0.8	–12.2	0.2420	11.3	xx	0.715773	xx	xx	0.77
KLX03A	964.50	975.15	10074	2005-02-07	–94.0	<0.8	–12.2	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10075	2005-02-10	–93.6	<0.8	–12.1	–	10.5	xx	0.715762	xx	xx	0.55
KLX03A	964.50	975.15	10076	2005-02-14	–94.8	<0.8	–12.2	0.2416	11.1	xx	0.715774	xx	xx	0.61
KLX03A	964.50	975.15	10077	2005-02-14	–	–	–	–	–	–	–	–	–	–

– = Not analysed

A = results will be reported later

xx = No result due to analytical problems

xxx = No result due to problem with the postal service.

< “value” = result less than detection limit

SICADA: h_o_isotopes, b_s_cl_sr_isotopes, c_s_isotopes

Table 10-3. Trace elements. Compilation November 2005.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	U ug/L	Th ug/L	Ars ug/L	Sc ug/L	Cd ug/L	Hg ug/L	V ug/L	Rb ug/L	Y ug/L	Zr ug/L	In ug/L	Cs ug/L	Ba ug/L	La ug/L	Hf ug/L
KLX03A	193.50	198.37	7948	2004-12-01	0.641	0.083	0.12	<0.05	<0.002	<0.002	4.57	6.05	0.720	3.81	<0.05	0.430	59.0	0.156	0.0387
KLX03A	193.50	198.37	7950	2004-12-06	0.636	0.081	0.14	0.053	<0.002	0.0027	4.98	6.01	0.730	3.90	<0.05	0.411	58.9	0.161	0.0398
KLX03A	193.50	198.37	7952	2004-12-13	0.658	0.102	0.27	0.060	0.0099	<0.002	4.84	7.02	0.698	4.05	<0.05	0.379	57.0	0.152	0.0430
KLX03A	193.50	198.37	7953	2004-12-15	0.631	0.104	0.24	0.057	0.0102	<0.002	4.74	6.78	0.680	3.94	<0.05	0.343	57.1	0.155	0.0390
KLX03A	193.50	198.37	7954	2004-12-15	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10085	2005-02-24	0.498	0.0430	0.19	<0.05	0.0778	<0.002	3.29	12.5	0.390	1.81	<0.05	0.343	91.8	0.0739	0.0152
KLX03A	408.00	415.30	10090	2005-03-17	0.404	0.0364	0.16	<0.05	<0.002	<0.002	2.59	12.1	0.363	1.57	<0.05	0.349	80.5	0.0883	0.0103
KLX03A	408.00	415.30	10091	2005-03-22	0.421	0.0402	0.14	<0.05	<0.002	<0.002	3.19	11.6	0.379	1.75	<0.05	0.358	79.5	0.0842	0.0135
KLX03A	408.00	415.30	10183	2005-03-22	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10194	2005-04-15	0.215	<0.04	0.26	<0.08	<0.004	<0.002	0.896	32.0	0.165	0.461	<0.04	0.875	166	0.0370	0.0045
KLX03A	735.50	748.04	10241	2005-04-22	0.143	<0.4	<1	<0.8	<0.04	<0.002	0.492	37.2	0.260	0.785	<0.4	1.19	172	<0.04	<0.04
KLX03A	735.50	748.04	10242	2005-04-25	0.127	<0.4	<1	<0.8	<0.04	<0.002	0.506	38.3	0.275	0.438	<0.4	1.22	175	<0.04	<0.04
KLX03A	735.50	748.04	10243	2005-04-25	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10007	2005-01-27	<0.01	<0.2	<1	<0.5	<0.05	<0.002	0.471	43.8	0.315	<0.3	<0.5	4.19	111	<0.05	<0.05
KLX03A	964.50	975.15	10009	2005-02-04	<0.01	<0.2	<1	<0.5	<0.05	<0.002	0.447	45.7	0.349	<0.3	<0.5	4.12	110	<0.05	<0.05
KLX03A	964.50	975.15	10076	2005-02-14	<0.01	<0.2	<1	<0.5	<0.05	<0.002	0.274	46.2	0.323	<0.3	<0.5	4.27	110	<0.05	<0.05
KLX03A	964.50	975.15	10077	2005-02-14	–	–	–	–	–	–	–	–	–	–	–	–	–	–	–

Table 10-3. Continue.

Idcode	Secup m	Seclow m	Sample no.	Tl ug/L	Ce ug/L	Pr ug/L	Nd ug/L	Sm ug/L	Eu ug/L	Gd ug/L	Tb ug/L	Dy ug/L	Ho ug/L	Er ug/L	Tm ug/L	Yb ug/L	Lu ug/L
KLX03A	193.50	198.37	7948	<0.03	0.343	0.0502	0.3030	0.0677	0.0153	0.0922	<0.05	0.0856	0.0201	0.0680	0.0100	0.0710	0.0138
KLX03A	193.50	198.37	7950	<0.03	0.364	0.0539	0.5650	0.0673	0.0147	0.0996	<0.05	0.0883	0.0213	0.0706	0.0106	0.0704	0.0133
KLX03A	193.50	198.37	7952	<0.03	0.316	0.0510	0.3400	0.0630	0.0180	0.1030	0.0120	0.0840	0.0220	0.0650	0.0110	0.0770	0.0160
KLX03A	193.50	198.37	7953	<0.03	0.309	0.0470	0.2990	0.0630	0.0180	0.1000	0.0130	0.0900	0.0240	0.0730	0.0120	0.0800	0.0140
KLX03A	193.50	198.37	7954	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	408.00	415.30	10085	<0.03	0.155	0.0252	0.339	0.0323	0.0127	0.0490	<0.05	0.0447	0.0118	0.0388	0.0055	0.0415	0.0089
KLX03A	408.00	415.30	10090	<0.03	0.175	0.0265	0.208	0.0315	0.0114	0.0425	<0.05	0.0423	0.0101	0.0347	0.0054	0.0412	0.0079
KLX03A	408.00	415.30	10091	<0.03	0.168	0.0246	0.210	0.0340	0.0108	0.0429	<0.05	0.0426	0.0113	0.0401	0.0056	0.0417	0.0081
KLX03A	408.00	415.30	10183	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	735.50	748.04	10194	<0.02	0.0534	0.0067	0.278	0.0102	0.0098	0.0140	<0.004	0.0120	<0.004	0.0122	<0.004	0.0172	<0.004
KLX03A	735.50	748.04	10241	<0.2	0.0508	<0.04	0.0914	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04
KLX03A	735.50	748.04	10242	<0.2	<0.04	<0.04	0.0851	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04	<0.04
KLX03A	735.50	748.04	10243	–	–	–	–	–	–	–	–	–	–	–	–	–	–
KLX03A	964.50	975.15	10007	<0.3	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
KLX03A	964.50	975.15	10009	<0.3	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
KLX03A	964.50	975.15	10076	<0.3	<0.05	<0.05	0.0567	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05
KLX03A	964.50	975.15	10077	–	–	–	–	–	–	–	–	–	–	–	–	–	–

– = Not analysed

A = Results will be reported later

x = No result due to sampling problems

xx = No result due to analytical problems

< “value” = result less than detection limit

SICADA: trace_elements

Table A10-4. Isotopes II (U-, Th, Ra- and Rn-isotopes). Compilation November 2005.

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
KLX03A	193.50	198.37	7948	2004-12-01	<50	<50	70	<50	<50	0.20	68.5
KLX03A	193.50	198.37	7950	2004-12-06	<50	<50	60	<50	<50	<0.10	57.4
KLX03A	193.50	198.37	7952	2004-12-13	<50	<50	<50	<50	<50	0.10	63.1
KLX03A	193.50	198.37	7953	2004-12-15	<50	50	50	<50	<50	<0.10	57.9
KLX03A	193.50	198.37	7954	2004-12-15	–	–	–	–	–	0.10	50.7
KLX03A	408.00	415.30	10085	2005-02-24	<50	<50	<50	<50	<50	1.00	19.2
KLX03A	408.00	415.30	10090	2005-03-17	<50	<50	<50	<50	<50	1.00	9.90
KLX03A	408.00	415.30	10091	2005-03-22	<50	<50	<50	<50	<50	1.00	15.5
KLX03A	408.00	415.30	10183	2005-03-22	–	–	–	–	–	<1.00	12.8
KLX03A	735.50	748.04	10194	2005-04-15	<50	<50	<50	<50	<50	–	–
KLX03A	735.50	748.04	10241	2005-04-22	<50	<50	<50	<50	<50	0.10	14.6
KLX03A	735.50	748.04	10242	2005-04-25	<50	<50	<50	<50	70	0.20	20.9
KLX03A	735.50	748.04	10243	2005-04-25	–	–	–	–	–	0.20	20.5
KLX03A	964.50	975.15	10007	2005-01-27	<50	<50	<50	<50	<50	1.10	33.0
KLX03A	964.50	975.15	10009	2005-02-04	<50	<50	<50	<50	<50	–	–
KLX03A	964.50	975.15	10075	2005-02-10	<50	<50	<50	<50	<50	1.20	32.2
KLX03A	964.50	975.15	10076	2005-02-14	<50	<50	<50	<50	<50	1.30	29.0
KLX03A	964.50	975.15	10077	2005-02-14	–	–	–	–	–	1.20	28.4

– = Not analysed

A = Results will be reported later

x = No result due to sampling problems

xx = No result due to analytical problems

< “value” = result less than detection limit

SICADA: u_th_isotope_t, ra_rn_isotope_t

Table A10-5. Dissolved gases. Compilation November 2005.

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_2H_6 µL/L	C_2H_4 µL/L	C_2H_2 µL/L	C_3H_8 µL/L	C_3H_6 µL/L	DISS_GAS mL/L H_2O
KLX03A	193.50	198.37	7953	2004-12-16	0.77	0.07	54	1.4	0.87	4.5	<1.9	<3.1	0.08	0.17	<0.05	<0.06	<0.06	62
KLX03A	408.00	415.30	10091	2005-03-22	0.73	0.72	49	1.8	0.62	0.46	110	–	0.1	0.07	<0.05	<0.05	<0.05	53
KLX03A	735.50	748.04	10242	2005-04-26	0.89	3.8	60	0.38	0.21	0.25	190	<3.3	0.42	0.12	<0.05	0.08	0.08	66
KLX03A	964.50	975.15	10076	2005-02-16	1.0	8.6	67	<2.3	0.06	0.13	<2.3	–	1.1	0.62	0.57	0.28	0.28	76

– = Not analysed

A = Results will be reported later

x = No result due to sampling problems

xx = No result due to analytical problems

< "value" = result below detection limit

SICADA: Dissolved_gases