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Oskarshamn site investigation

Complete chemical characterisation in KLX17A

**Results from two investigated borehole
sections: 416.0–437.5 m, 642.0–701.1 m**

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Geosigma AB

October 2008

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

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Abstract

Complete chemical characterisation is the most extensive chemical investigation method performed in core drilled boreholes. The method entails pumping, measurements on-line and water sampling for chemical analyses in isolated borehole sections during approximately three weeks per section at a flow rate of between 50 and 270 mL/min.

This report presents results from two sections in borehole KLX17A at 416.0–437.5 m borehole length (vertical depth 360–380 m) and 642.0–701.1 m borehole length (vertical depth 550–600 m). The results obtained include on-line measurements of redox potential, pH, dissolved oxygen, electrical conductivity and water temperature in the borehole sections together with chemical analyses of major constituents, trace metals and isotopes as well as gas content and composition. Furthermore, inorganic and organic colloids were investigated by fractionation, laser-induced breakdown colloid detection (LIBD) and scanning electron microscopy (SEM).

The water composition in section 642.0–701.1 m was stable during the pumping and sampling period, while there was a slight increasing concentration trend in section 416.0–437.5 m. The chloride concentrations amounted to approximately 590 mg/l in section 416.0–437.5 m and 18 mg/l in section 642.0–701.1 m while the flushing water contents were low; 1.7% and 0.2%, respectively. Enhanced concentrations of ^3H were found in some of the groundwater samples from both sections. The reason for this was likely contamination with de ionised water containing ^3H from the hydraulic pumping system as well as insufficient turnover time before sampling.

The redox potentials for the electrodes stabilised at about -300 mV in both sections.

In section 416.0–437.5 m, the colloid content measured by LIBD and SEM amounted to 110–240 $\mu\text{g/l}$ and 96 $\mu\text{g/l}$, respectively. The colloid content in the sample from section 642.0–701.1 m was too high to determine by LIBD technique, while the colloid concentration from the fractionation sample was 165 $\mu\text{g/l}$. The colloidal particles mainly consisted of aluminium, silicon (alumino-silicates, silicates), fluoride and iron.

Sammanfattning

Fullständig kemikaraktisering är den mest omfattande kemiska undersökningsmetoden för kärnborrhål. Metoden 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 270 mL/min.

Denna rapport presenterar resultat från två sektioner i borrhålet KLX17A vid 416,0–437,5 m borrhålslängd (vertikalt djup 360–380 m) och vid 642,0–701,1 m borrhålslängd (vertikalt djup 550–600 m). Resultaten omfattar mätningar on-line av redox potential, pH, löst syre, elektrisk konduktivitet och vattentemperatur i borrhålssektionen liksom kemiska analyser av huvudkomponenter, spårelement och isotoper samt bestämning av gasinnehåll och sammansättning. Vidare undersöktes oorganiska och organiska kolloider (humus och fulvosyror) med fraktioneringsteknik, detektering genom laserinducerad nedbrytning (LIBD) och svepelektronmikroskopi (SEM).

Vattensammansättningen i sektionen 642,0–701,1 m var relativt stabil under pump/provtagningens perioden medan sammansättningen i sektion 416,0–437,5 m uppvisade en något ökande trend. Kloridkoncentrationerna uppgick till ca 590 mg/l i sektion 416,0–437,5 m och ca 18 mg/l i sektion 642,0–701,1 m medan spolvattenhalterna var låga; 1,7 % respektive 0,2 %. Förhöjda ³H koncentrationer uppmättes i båda sektionerna. Orsaken till detta är sannolikt kontaminering av tritierat vatten från borrhålpumpens hydrauliska system samt otillräcklig omsättningstid av vattnet innan provtagning.

Redoxpotentialerna för elektroderna i båda sektionerna stabiliserade sig på ca –300 mV.

I sektion 416,0–437,5 m uppgick koncentrationen av kolloider mätt med LIBD och SEM till 110–240 µg/l respektive 96 µg/l. I sektion 642,0–701,1 m var kolloidkoncentrationen i provet som analyserades med LIBD för hög för att kunna bestämmas, medan resultatet från fraktioneringen gav en koncentration på 165 µg/l. De kolloidala partiklarna bestod till största delen av aluminium, kisel (alumino-silikater, silikater), fluor och järn.

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1 Introduction

This document reports performance of and results from the activity *Complete hydrochemical characterisation* in the cored borehole KLX17A performed within the site investigation at Oskarshamn /1/. The work was conducted according to the activity plan AP PS 400-06-138. The report presents hydrogeochemical data from field work carried out during the period of January to April 2007.

The controlling documents for the activity are listed in Table 1-1. The activity plan, the method description and the measurement system descriptions constitute SKB's internal controlling documents. The obtained data from the activity are reported to the SICADA database and are traceable by the activity plan number. Sampling for microbe studies was also performed within the present activity in both sections. The microbe investigations have been reported in a separate primary data report /2/.

Borehole KLX17A is a 701.1 m long telescopic borehole drilled at Laxemar and inclined 61° from the horizontal plane. The interval 0–65 m is percussion drilled with a diameter of 200 mm and the interval 65–701 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 KLX17A. The location of KLX17A is shown in Figure 1-1. The borehole design of KLX17A is presented in Appendix 1. 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 outlined in MD 600.004 (Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning).

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

Activity plan	Number	Version
Fullständig kemikaraktärisering med mobilt fältlaboratorium i KLX17A.	AP PS 400-06-138	1.0
Method description	Number	Version
Metodbeskrivning för fullständig kemikaraktärisering med mobilt fältlaboratorium.	SKB MD 430.017	2.0
Measurement system descriptions		
Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning.	SKB MD 600.004	1.0
Mätssystembeskrivningar för mobil kemienhet allmän del, slangvagn, borrhålsutrustning, mobil ytChemmac och dataapplikation.	SKB MD 434.004	1.0
	SKB MD 434.005	1.0
	SKB MD 434.006	1.0
	SKB MD 434.007	1.0
	SKB MD 434.018	
Mätssystembeskrivning för fraktionering av humus- och fulvosyror.	SKB MD 434.043	1.0
Mätssystembeskrivning för uppkoncentrering av humus- och fulvosyror.	SKB MD 434.044	1.0
Mätssystembeskrivning för kolloidfiltreringssystem	SKB MD 431.045	In progress
Instructions		
Provtagning och analys-kemilaboratorium	SKB MD 452.001-019	–

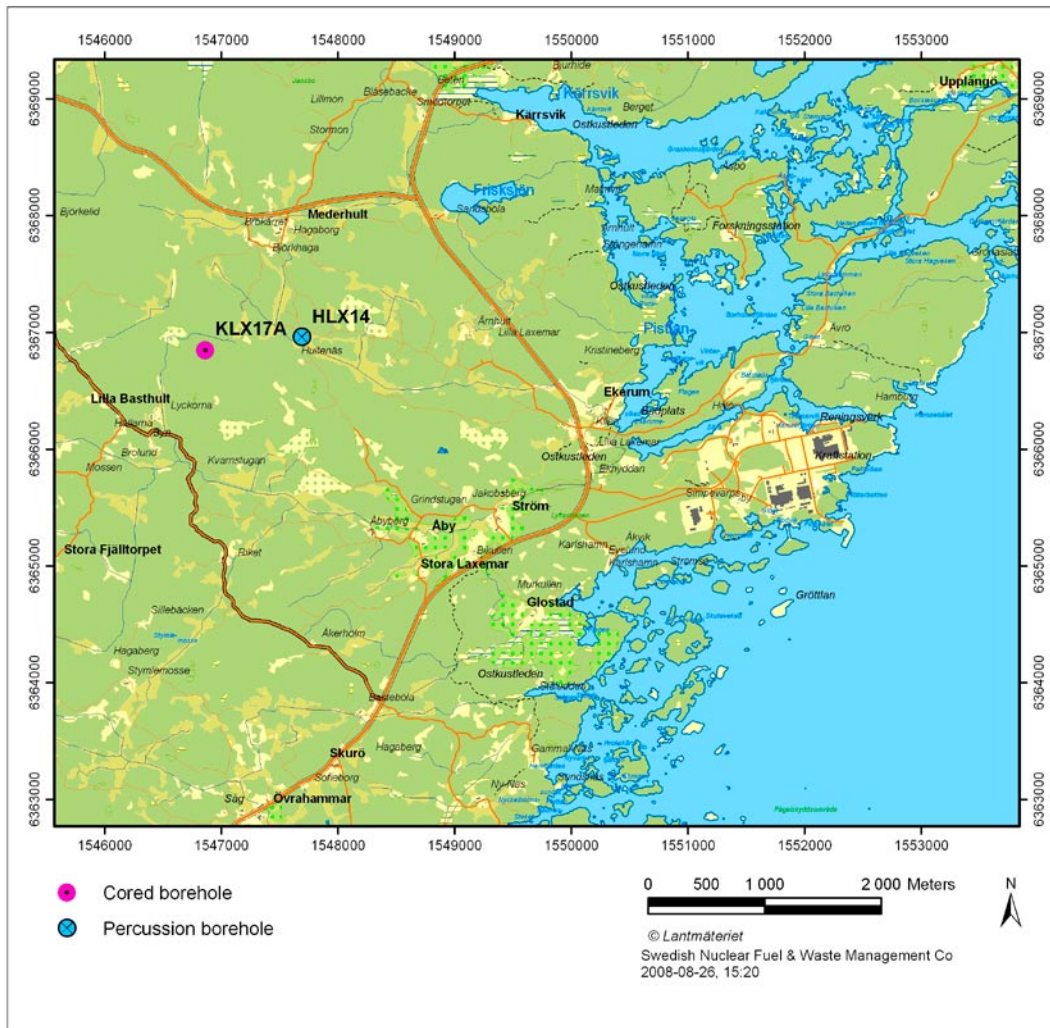


Figure 1-1. Locations of the core drilled borehole KLX17A and the percussion borehole HLX14, which served as the source of flushing water for the drilling of KLX17A, within the site investigation at Oskarshamn.

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 ground waters from other fracture systems.

The analytical programme was carried out according to SKB chemistry class 4 and class 5 including all options /1/. Furthermore, pH, redox potential (Eh) and water temperature were measured in flow-through cells downhole as well as at the ground surface. The flow-through cell at the surface also measured electrical conductivity and dissolved oxygen. In addition, samples were collected in situ in borehole sections for determination of gas content and composition, microbe content and their characterisation as well as for determination of colloid content by fractionation, LIBD and SEM and ICP-MS techniques. Fractionation of organic acids and inorganic species were performed in order to investigate size distribution (DOC and ICP analyses), and enrichment of organic acids was conducted in order to determine $\delta^{13}\text{C}$ and ^{14}C (pmC; percent modern carbon) in organic constituents.

3 Background

3.1 Flushing water history

The core drilling of the 701.1 m long borehole consumed 626 m³ of flushing water and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 1,079 m³.

Uranine was added automatically to the tank with flushing water that supplies flushing water to the drilling head. The Uranine concentration in the flushing water and returned water was checked regularly and a total of 87 samples of each sample type were analysed. The Uranine concentrations in the flushing water and in the returned water are presented in Figure 3-1. A water budget, presenting the amount of Uranine added to the borehole via the flushing water and the estimated amount recovered in the return water, is given in Table 3-1.

Table 3-1. Amount of Uranine added to KLX17A via the flushing water during core drilling and the amount recovered from the air-lift pumping.

Uranine	(g)
Added, calculated from the average Uranine concentration added and the total volume of flushing water.	137
Recovered, estimated from the average Uranine concentration recovered and the total volume of returned water.	158

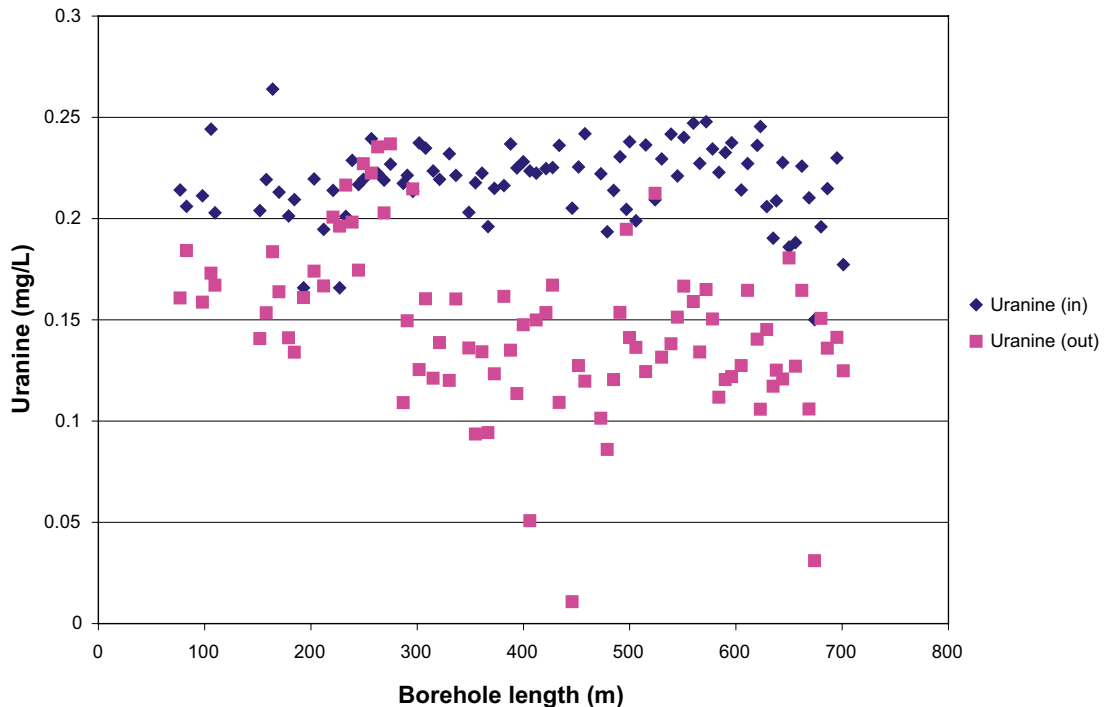


Figure 3-1. Uranine concentrations in the flushing water and in the recovered water versus borehole length.

The Uranine budget in Table 3-1 suggests that no flushing water has been lost to the borehole and the adjacent host bedrock during drilling, which is unusual. As a higher amount of Uranine cannot be recovered from the borehole than added to it, the calculation using average values has in this borehole resulted in an unacceptably high unreliability.

Detailed information on the flushing water and drilling of the borehole can be obtained from the drilling report /3/.

3.2 Previous activities in the borehole

KLX17A is a SKB chemistry-type core borehole intended for *Complete chemical characterisation*. Only activities that are necessary in order to select borehole sections are carried out in the borehole prior to the chemistry campaign. The more downhole equipment used in the borehole, the greater is the risk of contamination and effects on, for example, the in situ microbiological conditions. The activities/investigations performed in KLX17A prior to the chemistry campaign are listed in Table 3-2 below.

3.3 Choice of borehole sections

The main objective for the *complete chemical characterisation* in KLX17A was to investigate groundwater at repository depth (c. 400–550 m). Three borehole sections were selected that fulfilled two or three of the following criteria;

- flow yield > 10, 000 mL/h
- near repository depth
- suitable for the positioning of the packers

Section 642–701 m was selected because of its location near repository depth (borehole inclination 61%). In addition, sections 416–437 m and 313–316 m were selected. For the investigated sections 642–701 m and 416–437 m there were no single fractures with sufficient flow yield and therefore several water bearing fracture zones were included. The pumping was carried out without any significant drawdown in neither of the two sections.

Table 3-2. Activities performed in KLX17A prior and in connection to the chemical characterisation.

Activity	Date of completion	Length or section (m)	Comment
Percussion drilling	2006-08-15	0.15–65.42	
Core drilling	2006-10-23	65.42–701.08	
BIPS-logging	2006-11-30	0.00–696.78	/4/
Geophysical logging	2006-11-14	2.30–700.50	/5/
Difference flow logging	2007-01-08	2.60–701.08	/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 downhole (borehole Chemmac).

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

The mobile units used for the investigation of borehole KLX17A consisted of the hose unit S2, the laboratory unit L2 and the computer unit MYC 2 including surface Chemmac.



Figure 4-1. The mobile units used at KLX17A; from left container for collecting the water from the borehole, laboratory unit, hose unit with downhole equipment and a unit for computer work.

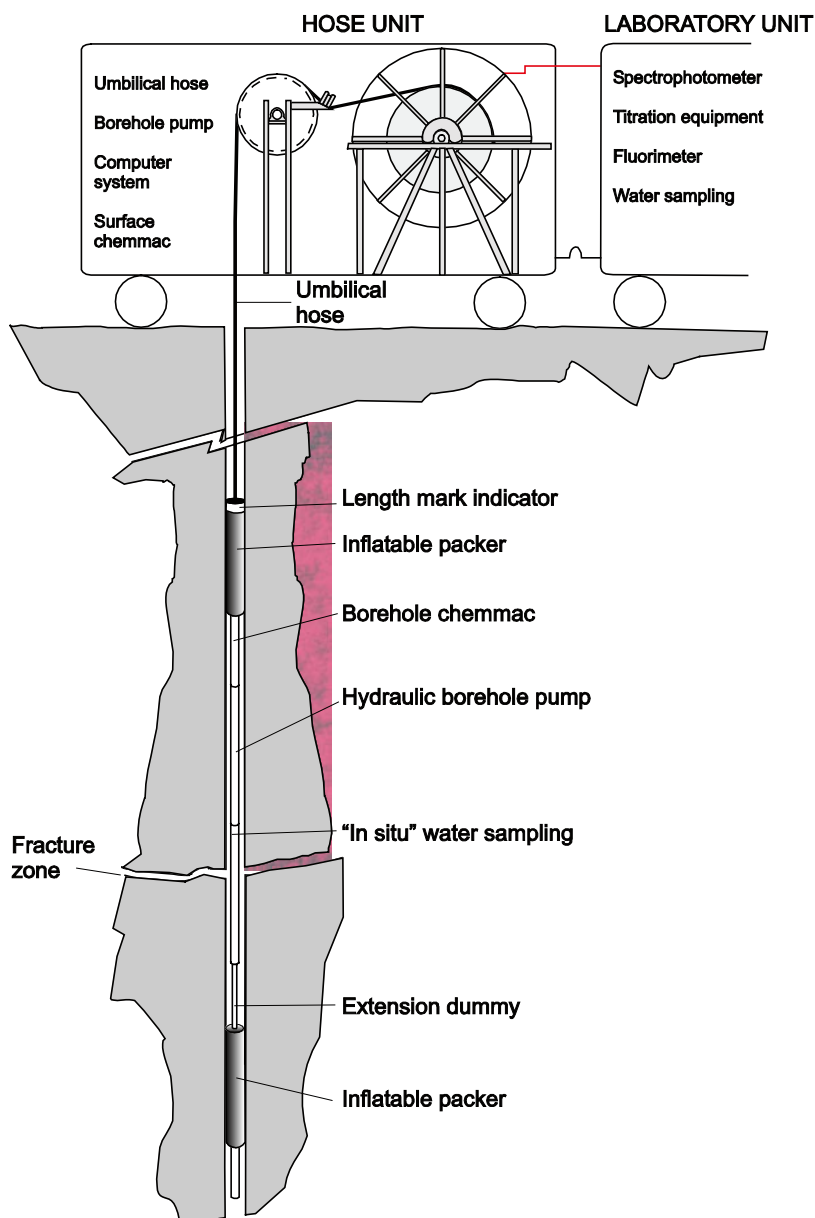


Figure 4-2. The mobile laboratory including laboratory unit, hose unit and downhole equipment. The configuration of the downhole units in the borehole can be varied depending on desired section length. However, the in situ water sampler must always be positioned first in the sample water path.

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 equipment is described in SKB MD 431.045 (Mätssystembeskrivning för kolloidfiltrerings-system, handhavandel (SKB internal controlling document to be published)). Note that the pore sizes of the five connected filters have been changed to 2, 2, 0.4, 0.2 and 0.05 μm . The pore sizes have been reduced because previous analyses have indicated an absence of large colloidal particles. Figure 4-3 shows the equipment setup.

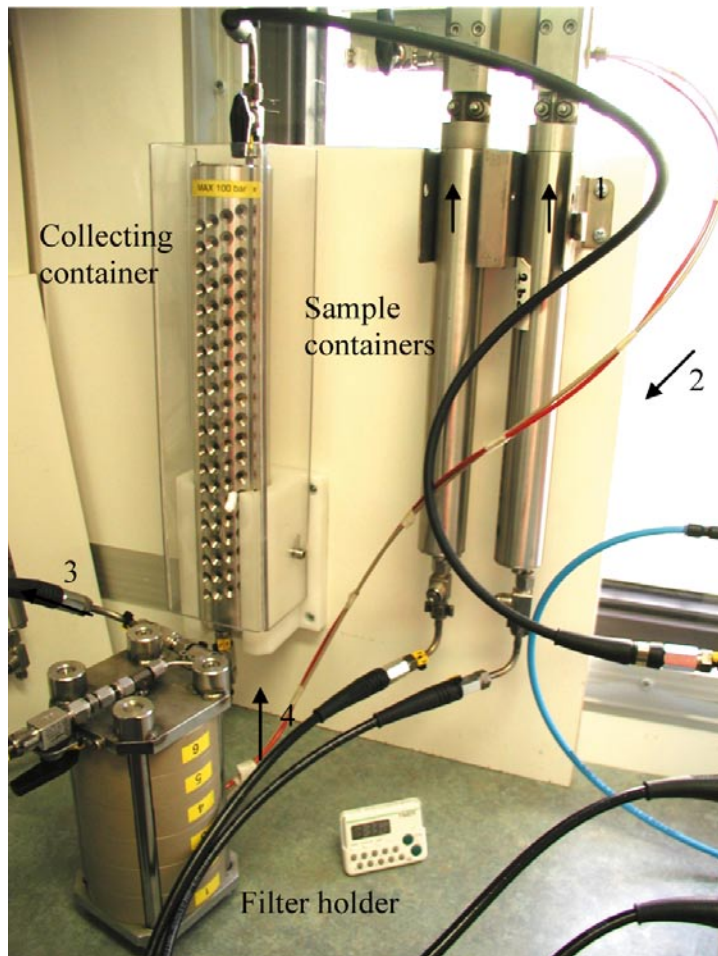


Figure 4-3. The colloid filtering equipment including the sample containers, the filter holder package and the collecting container. The black arrows, 1 to 4, show the flow direction of the sample water through the system.

The major equipment features are:

- Filtering is performed in a closed system under an argon atmosphere, thus avoiding the risk of iron precipitation due to contact between the groundwater sample and air.
- Filtering is performed at a pressure similar to that of the groundwater in the borehole section. The system is adjusted to create a pressure difference between the inlet of the filter package and the outlet side. The pressure difference drives the sample water through the filters.
- The design of the sample containers, and the mounting with the outlet at the top, prevents migration of larger particles that might clog the filters. Furthermore, clogging is prevented by the first two filters with pore sizes 2 μm which are mounted parallel to each other.

A source of possible contamination is the PVB sample containers that are made of stainless steel. An improvement could be to use Teflon coating on the insides of the cylindrical containers.

When performing the filtration prior to a colloid study by SEM (Scanning Electron Microscopy), the equipment is supplemented with a portable glove-box, filled with argon for handling of the filters containing the oxygen-sensitive colloids.

4.3 Equipment for enrichment of humic and fulvic acids

Enrichment of humic and fulvic acids is conducted in order to collect enough material to determine $\delta^{13}\text{C}$ and ^{14}C (pmC) 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 (Mätssystembeskrivning för uppkoncentrering av humus- och fulvosyror, SKB internal controlling document). Figure 4-4 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 (Mätssystembeskrivning för fraktionering av humus- och fulvosyror, SKB internal controlling document). Figure 4-5 shows the equipment setup and Figure 4-6 schematically describes the function of a membrane.

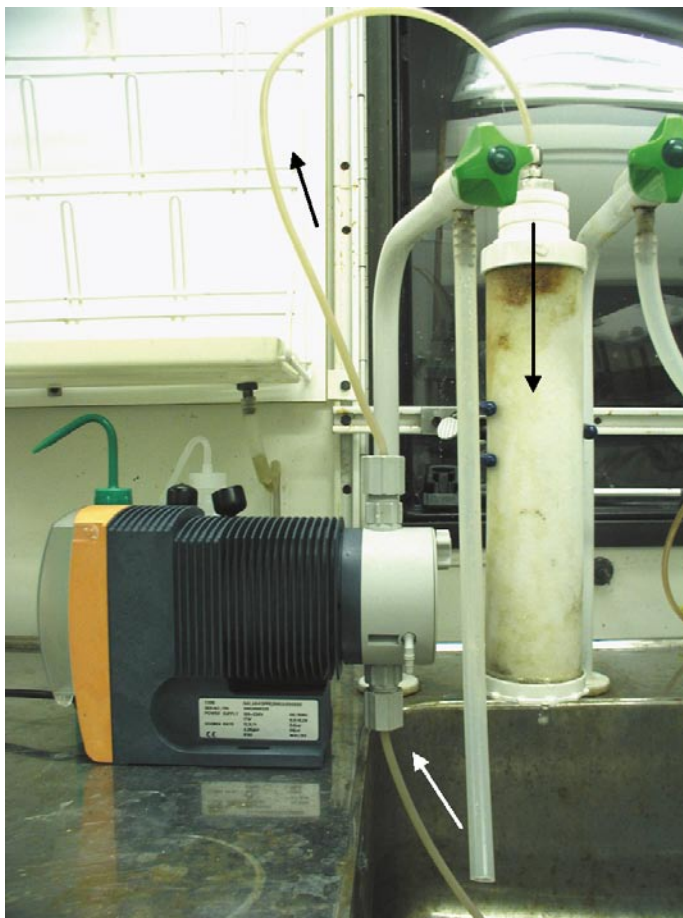


Figure 4-4. The ion exchange column. The arrows show the water flow direction.

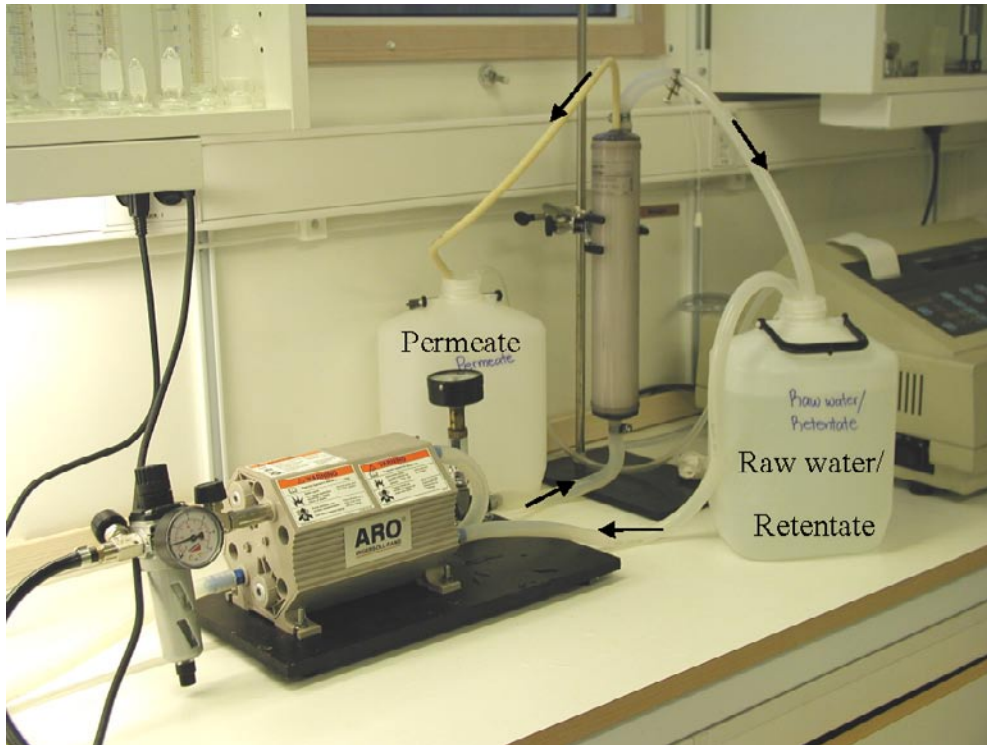


Figure 4-5. Equipment for fractionation of humic and fulvic acids.

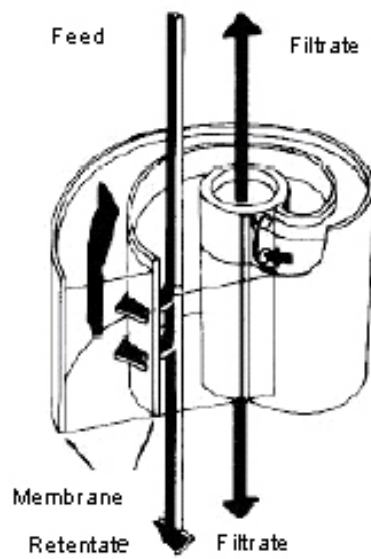


Figure 4-6. Outline of membrane filter with water flow directions.

5 Performance

5.1 General

Chemical characterisation in borehole KLX17A was conducted according to activity plan AP PS 400-06-138 following the method described in SKB MD 430.017 (Metodbeskrivning för fullständig karakterisering med mobilt fältlaboratorium). Table 5-1 gives an overview of the investigation sequence in KLX17A.

5.2 Chemical characterisation

5.2.1 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. Preparations 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 on the outside using 70% denatured ethanol and on the inside using chlorine dioxide. One of the containers is used for microbe sampling and sterile conditions are desirable. The containers are purged with nitrogen gas and a small nitrogen gas pressure is maintained in the containers. The magnitude of the pressure depends on the depth of the section to be sampled.
- Calibration of the pH and redox electrodes in the borehole Chemmac.

The different downhole units are assembled during lowering 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.

Table 5-1. Investigation sequence in KLX17A.

Start date/ Stop date	Section (m)	Comment
2007-01-30/ 2007-03-01	642.00–701.08	Pumped volume = 11.2 m ³ Flow rate approx. 270 mL/min
2007-03-02/ 2007-04-24	416.00–437.51	Pumped volume = 15.2 m ³ Flow rate approx. 230 mL/min

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

- Calibration of the pH and redox electrodes as well as the electrical conductivity and oxygen sensors in the surface Chemmac is conducted when the pumped water from the borehole section has reached the surface.
- Careful attention is paid to ensure that the packed off section is well isolated from the rest of the borehole. A significant drawdown in the section during pumping is one indication that the section is properly sealed off. Leakage would cause pumping of water from the borehole column above and/or below the packers and not only from the fracture zone of interest. However, the drawdown in the borehole section must not be too large, because the greater the drawdown, the larger the bedrock volume affected by the pumping and the risk of mixing with groundwater from other shallower and/or deeper fracture systems increases. The pumping flow rate is adjusted depending on the flow yield from the fracture or fracture zone (to between 50 and 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 pH conductivity measurements and by immediate analyses (pH, Uranine, chloride, alkalinity, ammonium, ferrous and total iron).
- 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 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.

The following sections (5.2.2–5.2.3) shortly describe the performance in each section.

The main activities are presented in the events tables together with SKB sample numbers of the corresponding water samples.

5.2.2 Performance in section 416.0–437.5 m

The chemical characterisation in section 416.0–437.5 m was performed using the following configuration of the downhole equipment in the borehole. From the top: umbilical hose, length mark detector, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP), extension and lower packer, see Appendix 4. The pressures above and within the section were measured by the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping flow rate was about 230 mL/min and the drawdown insignificant at the end of the measurement period. The turnover time corresponds to 1 day at the current flow rate and the turnover was in total 40 times at the end of the investigation period. Diagrams showing the pressures above and within the borehole section and the flow rate during the pumping/measurement period are presented in Appendix 5. The events during the investigation are listed in Table 5-2.

Table 5-2. Events during the pumping/measurement period in section 416.0–437.5 m.

Date	Event	Sample no.
070301	Calibration of borehole Chemmac and surface Chemmac. Exchange of oxygen electrode.	
070302	Lowering of downhole equipment S2 (416.00–437.51 m) Start of borehole pump and Chemmac measurements	
070305	Water sampling: Uranine	11763
070306	Water sampling: SKB class 2	11764
070308	Alarm regarding low water flow.	
070309	Lifting Replacement of broken spring in the borehole pump. Lowering of downhole equipment S2 (416.00–437.51 m) Start of borehole pump and Chemmac measurements	
070312	Water sampling: SKB class 5 The sample for U and Th is stored in the archive The current to the borehole Chemmac is switched off due to high current consumption. Restart of the measurement application.	11765
070313	Humic and fulvic acids; enrichment start	
070315	Water sampling: SKB class 4	11766
070319	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11767
070320	Humic and fulvic acids; fractionation 1,000 D Change of conductivity scale from 2,000 mS/m to 500 mS/m.	11810
070321	Water sampling: SKB class 5 The sample for U and Th is stored in the archive Humic and fulvic acids; fractionation 5,000 D	11768 11810
070323	Water sampling: SKB class 4	11769
070326	Lifting Alarm regarding low water flow. Replacement of broken spring in the borehole pump. Lowering of downhole equipment S2 (416.00–437.51 m) Start of borehole pump and Chemmac measurements	
070327	Lifting Leakage of water from the packers. Repair. Calibration of borehole Chemmac Lowering of downhole equipment S2 (416.00–437.51 m) Start of borehole pump and Chemmac measurements	
070328	Calibration of surface Chemmac	
070330	Water sampling: SKB class 4	11770
070402	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11771
070404	Water sampling: SKB class 4	11772
070410	Low water flow due to defective driving pump. Repair. Change of relay.	
070411	Water sampling: SKB class 1; pH, conductivity, alkalinity, chlorinity, Uranine, Cl ⁻ , Br ⁻ , F ⁻ and SO ₄ ²⁻	11773
070412	Water sampling: SKB class 5 The sample for U and Th is stored in the archive	11809
070416	Lifting Alarm regarding low water flow. Replacement of broken spring in the borehole pump. Lowering of downhole equipment S2 (416.00–437.51 m) Start of borehole pump and Chemmac measurements	

070418	Water sampling: SKB class 5; all options	11810
	Water sampling: SKB class 5, control sample. Density measurement	11811
	PVP-sampler: opening of valve at 17:24	
070419	PVP-sampler: closure of valve at 06:36	
	Residual current operated circuit breaker.	
	Humic and fulvic acids; enrichment stop	11810
	Lifting	
	Sampling for microbes and dissolved gases	11810
	Lowering of downhole equipment S2 (416.00–437.51 m)	
	Start of borehole pump and Chemmac measurements	
070423	Water sampling: SKB class 5	11812
	The sample for U and Th is stored in the archive	
	PVP-sampler: opening of valve at 14:22	
070424	PVP-sampler: closure of valve at 06:35	
	Sampling for colloids	11810
	End of Chemmac measurements	
	Lifting	
	Calibration of borehole Chemmac and surface Chemmac	

5.2.3 Performance in section 642.0–701.1 m

The chemical characterisation in section 642.0–701.1 m was performed using the following configuration of the downhole equipment in the borehole. From the top: umbilical hose, length mark detector, borehole Chemmac, upper packer, borehole pump, in situ water sampler (PVP), and lower packer, see Appendix 4. The pressures above and within the section were measured using the borehole Chemmac unit and the PVP water sampling unit, respectively.

The pumping flow rate was about 270 mL/min and the drawdown approximately 0.4 m at the end of the measurement period. The turnover time corresponds to 3 days at the current flow rate and the turnover was in total 10 times at the end of the investigation period. Diagrams showing the pressures above and within the borehole section and the flow rate during the pumping/measurement period are presented in Appendix 5. The events during the investigation are listed in Table 5-3.

Table 5-3. Events during the pumping/measurement period in section 642.0–701.1 m.

Date	Event	Sample no.
070129	Calibration of borehole Chemmac	
070130	Lowering of downhole equipment S2 (642.00–701.08 m)	
	Start of borehole pump and Chemmac measurements	
070131	Calibration of surface Chemmac. Cleaning of oxygen electrode with nitric acid and change of membrane.	
	Water sampling: SKB class 2	11612
070201	Water sampling: SKB class 4	11635
070205	Water sampling: SKB class 5	11684
	The sample for U and Th is stored in the archive	
070207	Humic and fulvic acids; enrichment start	
070208	Water sampling: SKB class 4	11688
070212	Water sampling: SKB class 5	11689
	The sample for U and Th is stored in the archive	

070213	<p>Possible leakage of water from the borehole pump. Filling of about 25 liters of water in the tank for the driving pump. Filling of water in the tank for the packers. No leakage in the packers could be observed.</p> <p>Change of maximum and minimum values in the measurement application for EREFB and ECB to $\pm 1,000$ mV, since the recorded values were out of range.</p>	
070214	<p>Driving pump turned off since the water level in the tank has decreased. Restarted driving water pump, the level was apparently decreasing slowly.</p>	
070215	<p>Driving pump turned off since the water tank was empty. Leaking borehole pump.</p> <p>Lifting</p> <p>Change of borehole pump</p> <p>Lowering of downhole equipment S2 (642.00–701.08 m)</p> <p>Start of borehole pump and Chemmac measurements</p>	
070216	<p>Alarm regarding low water flow. High current consumption and lost contact with borehole Chemmac. The current to the borehole Chemmac is switched off during the weekend.</p>	
070219	<p>Lifting</p> <p>Repair of electronic part in the coupling of the umbilical hose.</p> <p>Lowering of downhole equipment S2 (642.00–701.08 m)</p> <p>Start of borehole pump and Chemmac measurements</p>	
070221	<p>Water sampling: SKB class 5</p> <p>The sample for U and Th is stored in the archive</p> <p>The current to the borehole Chemmac is switched off due to high current consumption.</p>	11690
	<p>Humic and fulvic acids; fractionation 1,000 D</p>	11692
070222	<p>Humic and fulvic acids; fractionation 5,000 D</p>	11692
070223	<p>Water sampling: SKB class 4</p>	11691
070226	<p>Water sampling: SKB class 5; all options</p>	11692
070226	<p>Water sampling: SKB class 5; control sample. Density measurement</p> <p>Exchange of deionised water in pump system (tanks for driving pump and packers) and filter for deionised water in mobile laboratory (L2).</p> <p>PVP-sampler: opening of valve at 18:55</p>	11693
070227	<p>PVP-sampler: closure of valve at 06:51</p> <p>Sampling for colloids</p> <p>End of Chemmac measurements</p> <p>Humic and fulvic acids; enrichment stop</p> <p>Lifting</p> <p>Exchange of defective pH electrode EPHIB.</p> <p>Calibration of borehole Chemmac</p> <p>Lowering of downhole equipment S2 (642.00–701.08 m)</p> <p>Start of borehole pump and Chemmac measurements</p>	11692
070228	<p>Water sampling: SKB class 5</p> <p>PVP-sampler: opening of valve at 16:37</p>	11694
070301	<p>PVP-sampler: closure of valve at 06:40</p> <p>Sampling for microbes and gases</p> <p>End of Chemmac measurements</p> <p>Lifting</p> <p>Calibration of surface Chemmac</p>	

5.3 Water sampling, sample treatment and analyses

The pumped water from the borehole section is led 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 groundwater collected during one day and consists of several sample portions, labelled with the same sample number.

An overview of sample treatment and analysis methods is given in Appendix 10. The routines are applicable independently of sampling method or type of sampling object.

5.4 Collection of in situ water samples

The in situ water sampling was conducted successfully in both borehole sections. The sampling was repeated in order to obtain additional samples for colloid determination using LIBD in both sections (Appendix 8).

In addition, in section 416.0–437.5 m filters from colloid filtration was analysed by SEM. Dissolved gases were analysed by two independent laboratories. The purpose of each sample portion is given in Table 5-4 and 5-5.

The PVB containers were all quality controlled before use. This procedure includes de-assembling the container, thorough cleaning, re-assembling and measurement of piston friction. The filled PVB containers were packed together with ice packs in insulated bags and sent to the laboratories by express delivery service immediately after sampling.

Table 5-4. Collection and purpose of in situ water sample portions in section 416.0–437.5 m.

Sample portion no.	Section 416.0–437.5 m 2007-04-19	Section 416.0–437.5 m 2007-04-24
1	Dissolved gas (Lab 1), N ₂	Colloids (LIBD)
2	Dissolved gas (Lab 2), N ₂	Colloids (LIBD)
3	Microbes	Colloids (SEM)
4	–	–

Table 5-5. Collection and purpose of in situ water sample portions in section 642.0–701.1 m.

Sample portion no.	Section 642.0–701.1 m 2007-02-27	Section 642.0–701.1 m 2007-03-01
1	Colloids (LIBD)	Dissolved gas (Lab 1), N ₂
2	Colloids (LIBD)	Dissolved gas (Lab 2), N ₂
3	Colloids (filtration)	Microbes
4	Colloids (filtration)	–

5.5 Colloid filtration

The method for sampling of colloids in groundwater entails filtering of 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. One or two of the four sample portions collected in situ in each borehole section are used for colloid filtration, followed by analysis with two different methods (ICP-MS or SEM). Data on performance of the filtration runs are given in Table 5-6.

The general filtration method that normally is used to obtain colloid samples for ICP-MS determinations was somewhat modified prior to performance of the filtering intended for SEM studies. The most important stages are filtering of one instead of two PVB containers, flushing of the filters with de-ionised water and handling of the filters in argon atmosphere. The modifications are documented in the activity plan AP PF 400-07-029.

Each filtration results in five filter samples (two 2 µm, one 0.4 µm, one 0.2 µm and one 0.05 µm filter pore sizes) and two water samples (water in and water out). All samples from section 642.0–701.1 m and the water samples from “Filtration – SEM” (section 416.0–437.5 m) were sent for ICP-MS analyses (major constituents and common trace metals). In section 642.0–701.1 m, by mistake the filter pore sizes used were two 2 µm, one 0.2 µm and two 0.05 µm. In section 416.0–437.5 m, the 0.2 µm and 0.05 µm filters were sent for analyses by scanning electron microscopy (SEM) in a non diffusion plastic bag filled with argon.

A leakage test of the system at 10 bars was also done prior to the sampling in order to eliminate the risk of leakage. No leakage was detected and the system was dried and assembled. The filters used during the test were sent for analysis of metals as blank samples.

To check the validity of the approach, a test was performed using two different commercial Latex Microsphere Suspensions containing particles with pore sizes of 0.08 µm and 0.24 µm, respectively. The filters were weighed before and after filtering (and drying to stable weight) of a suspension containing 0.1 mg of each pore size, at a pressure of 10 bars. The weights increased on the 0.4 µm and 2.0 µm filters (on which neither of the commercial colloids should be present) and were rather high (0.03–0.09 mg). The weights on the 0.2 µm and 0.05 µm filters were also somewhat too high, 0.17 and 0.20 mg, respectively. Despite the weight increase that may be due to a minor water uptake, the test indicates that the total amount of synthetic colloids that passed through the tubing and valve system were collected on the intended filters.

Table 5-6. 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
416.0–437.5 m /20070324	~35	3.0	~14	12	108.5	Leakage test prior to filtration: no leakage was noticed.
642.0–701.1 m /20070227	~55	15	~16	140	177	Leakage test prior to filtration: no leakage was noticed. Due to the high diff. pressure, three of the filters were broken.

5.6 Enrichment of humic and fulvic acids

Enrichment of humic and fulvic acids was conducted in order to collect enough material to determine $\delta^{13}\text{C}$ and ^{14}C (pmC) in organic constituents in the groundwater. The method is described in SKB MD 431.044 (Mätsystembeskrivning för uppkoncentrering av humus- och fulvosyror). The enrichment method entails collection of organic acids on an ion exchanger, elution of the resin and evaporation of the resulting solution. The dry residue is used for isotope determination and a minimum amount of 10 mg organic carbon is needed. In addition to organic material, the residue also contains sodium hydroxide from the elution. The sample is acidified in order to prevent the formation of carbon dioxide.

Estimations of total duration and water volume through the ion exchanger for section 416.0–437.5 m are given in Table 5-7. The sample collected from section 642.0–701.1 m was unfortunately lost after completed sampling.

5.7 Fractionation of humic and fulvic acids

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

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 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 5-7. Enrichment time and water volume through the ion exchanger.

Borehole section [m]	Duration of enrichment [days]	Volume through ion exchanger [L]
416.0–437.5	33	1,560

5.8 Nonconformities

The *Complete chemical characterisation* in KLX17A has been conducted according to the SKB internal controlling documents AP PS 400-06-138 and SKB MD 430.017 with the following deviations and remarks:

- The flushing water content, 1.7%, in section 416.0–437.5 m slightly exceeded the allowed upper limit for flushing water content; 1%.
- The in situ sampling in both sections was repeated once in order to collect sample portions for analysis of colloids using Laser Induced Breakdown Detection (LIBD). Furthermore, dissolved gases were analysed by two independent laboratories.
- The filters from the colloid filtration in section 416.0–437.5 m were analysed by SEM.
- When performing the colloid filtration in section 642.0–701.1 m, by mistake the filter pore sizes used were two 2 µm filters, one 0.2 µm and two 0.05 µm filters. In addition, only one PVB container was filtered, as the second PVB container did not open despite a raised differential pressure.
- There were no results from the enrichment of humic and fulvic acids in section 642.0–701.1 m due to loss of the sample.
- Some equipment malfunctions were encountered during the investigation:
 - defective spring in borehole pump,
 - loss of connection with the borehole Chemmac,
 - leakage in borehole pump,
 - unfixed parts in the coupling of the umbilical hose.

6 Data handling and interpretation

6.1 Chemmac measurement data

The processing of Chemmac data are described in SKB MD 434.007-02 (Mätssystembeskrivning för Chemmac mätsystem, SKB internal controlling document, in progress).

6.1.1 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.

6.1.2 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.

6.2 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 $\pm 5\%$ are considered acceptable (in surface waters $\pm 10\%$).

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

- 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 6-1.

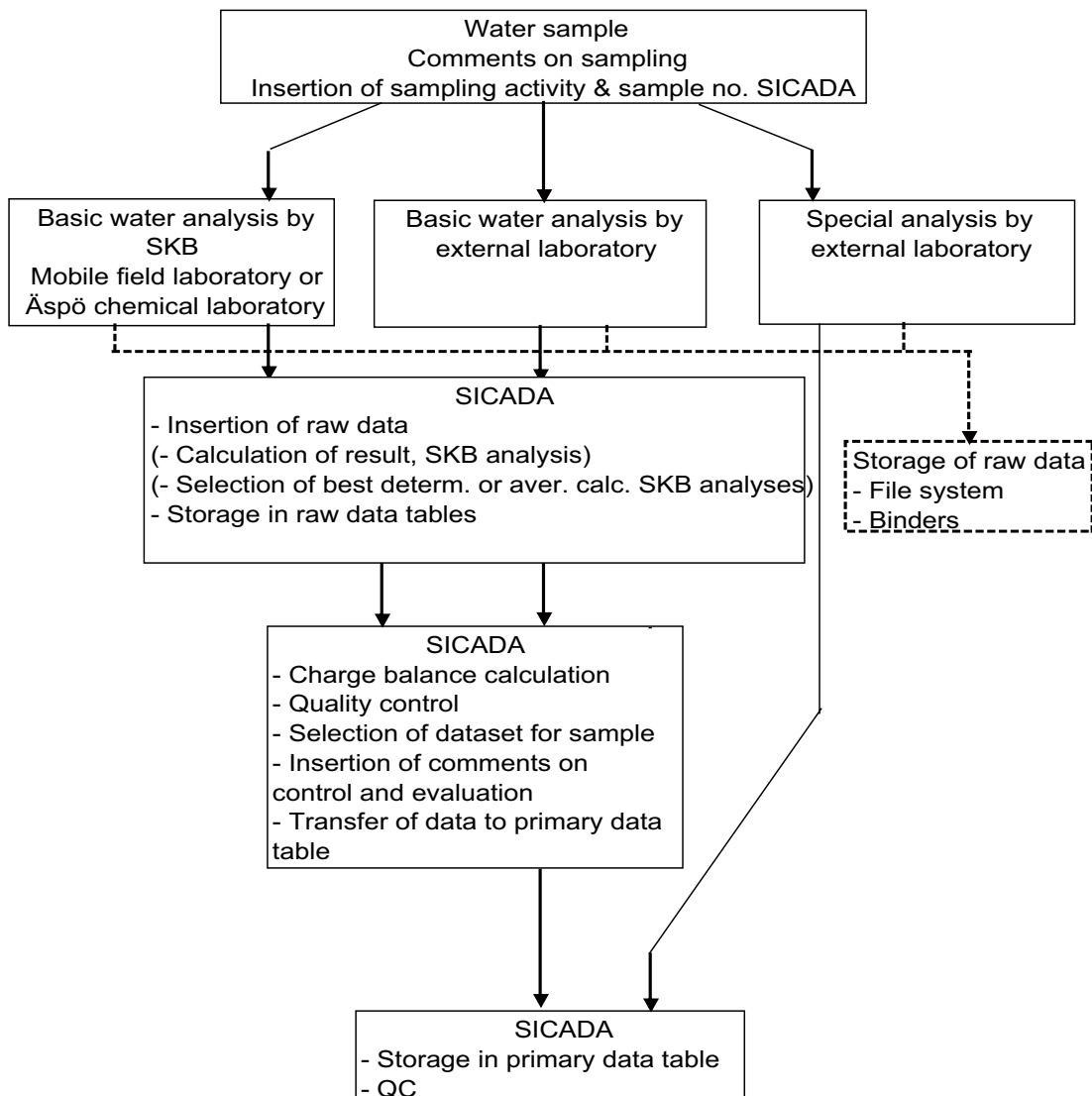


Figure 6-1. Overview of data management for hydrogeochemical data.

6.3 Data from special sampling methods

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

Separate sampling activities, methods and sample numbers are defined for data on dissolved gases, colloids, fractions of humic and fulvic acids and $\delta^{13}\text{C}$ and ^{14}C (pmC) determined on organic constituents. All analytical data are subjected to quality control and stored in the SICADA database.

6.3.1 Colloid filtration

The concentration of the colloid portion caught on each filter from the filtration followed by detection with ICP-MS 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 from the “sum” of the measurement uncertainties of the filter analyses and estimated volume error (volume passing through the filters) 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 [$\mu\text{g/L}$]
	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 results from water samples are directly inserted into the primary data tables in SICADA.

6.3.2 Dissolved gases

The results of the gas analyses are stored in the primary data tables in SICADA. The results for O_2 , N_2 and Ar from laboratory number 2 are recalculated to in order to be comparable to the results from laboratory number 1 that are uncorrected for air contamination. The gas results reported in SICADA correspond to values not corrected for air contamination.

6.3.3 Enrichment of humic and fulvic acids

The $\delta^{13}\text{C}$ and ^{14}C (pmC) values for enriched organic acids are stored in SICADA without processing or interpretation.

6.3.4 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, (Mätssystembeskrivning för fraktionering av humus- och fulvosyror). Comparison of the four concentration values from the two filters results in values for three fractions i.e. < 1,000 D, 1,000–5,000 D and > 5,000 D.

7 Results

Original data from the reported activity are stored in the primary database Sicada. Data are traceable in Sicada by the Activity Plan number (AP PS 400-06-138). Only data in databases are accepted for further interpretation and modelling. The data presented in this report are regarded as copies of the original data. Data in the databases may be revised, if needed. However, such revision of the database will not necessarily result in a revision of this report, although the normal procedure is that major data revisions entail a revision of P-reports. Minor data revisions are normally presented as supplements, available at www.skb.se.

7.1 Chemmac measurements

The data sequences of pH, Eh, electrical conductivity, oxygen and temperature values from the Chemmac measurements in borehole sections 416.0–437.5 m and 642.0–701.1 m are plotted versus time in Appendices 6 and 7 respectively. The measured time series were evaluated in order to obtain a representative value of pH, Eh, electrical conductivity and dissolved oxygen for the borehole as described in Section 6.1. Data were selected from the last part of the measured time series sequences (where the electrodes show stable values), marked with an arrow in the diagrams in the appendices. The evaluated results from the measurements in the investigated sections are given in Table 7-1 together with the corresponding results from the LIBD measurements.

Table 7-1. Evaluated results from the Chemmac and LIBD measurements in KLX17A.

Borehole section [m]	Electrical conductivity* [mS/m]	pH (borehole chemmac)**	pH (surface chemmac)**	Eh** [mV]	Dissolved oxygen*** [mg/L]
416.0–437.5	215 ± 6	8.0 ± 0.1	8.0 ± 0.2	-297 ± 13	0.00
416.0–437.5 PVB (LIBD)(1)****	224	–	8.1	-237 ^m	<0.029
416.0–437.5 PVB (LIBD)(2)****	220	–	7.94	-217 ^m	<0.015
642.0–701.1	46 ± 2	–	8.3 ± 0.2	-303 ± 8 ^s	–
642.0–701.1 PVB (LIBD)(1)****	51	–	8.45	-286 ^c	<0.002
642.0–701.1 PVB (LIBD)(2)****	58	–	8.39	-278 ^c	<0.001

*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 6.1.

*** Measurement interval 0–15 mg/L, resolution and measurement uncertainty ± 0.01 mg/L.

**** See Appendix 8.

^m = measured redox potential.

^s = only values from surface Chemmac have been used in the calculation.

^c = redox potential calculated with PHREEQC.

The redox potentials and pH of the electrodes in borehole and surface Chemmac were stable and consistent in section 416.0–437.5 m. In section 642.0–701.1 m the electrodes at the surface showed stable potentials, while the readings from the borehole electrodes were unreliable due to high consumption of current in borehole Chemmac. The recorded redox potentials from the on-line measurements were approximately –300 mV and in reasonable agreement with the calculated values from the LIBD experiment, while the measured redox potentials from the LIBD experiment were about 60–80 mV higher, which could be explained by the limited time of measurement. The pH was about 8 in both sections.

The response from the oxygen electrode in section 642.0–701.1 m was not reliable, probably due to a defective electrode, and the data was not reported to SICADA. After exchange of the electrode in section 416.0–437.5 m the recorded values were reasonable and agreeing with the measurements performed in connection to the LIBD experiment.

7.2 Water analyses

7.2.1 Basic water analyses

The basic water analyses include the major constituents Na, K, Ca, Mg, S, Sr, SO_4^{2-} , Cl^- , Si and HCO_3^- as well as the minor constituents Fe, Li, Mn, DOC, F, I, HS^- and NH_4^+ . Furthermore, batch measurements of pH (lab-pH) and electrical conductivity (lab-EC) 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 electrical conductivity are compared with the corresponding on-line Chemmac measurement values in Appendices 6 and 7.

The charge balance errors give an indication of the quality and uncertainty of the analyses of major constituents. The errors did exceed $\pm 5\%$ in one case, the second sample in the sample series from 642.0–701.1 m. for which the error was -5.8% . A comparison between results from different laboratories and methods shows that the agreement is acceptable in most cases; in general less than 10% for each analysed constituent.

The flushing water contents in the sample series collected from the borehole sections are presented in Figure 7-1. The flushing water content should not exceed 1% in order for a sample to be considered representative for the groundwater. This condition was met for samples collected in section 642.0–701.1 m, with flushing water contents of 0.2%, while the content in section 416.0–437.5 m was 1.7%. The flushing water content is calculated using the average Uranine concentration in the added flushing water during core drilling of the sampled fracture zone.

The concentration levels of sodium, calcium and chloride are presented in Figures 7-2 and 7-3. The concentrations of all major constituents remained more or less constant during the pumping and sampling period in section 642.0–701.1 m. The water was not completely turned over at the time for the first sample, which explains the deviating chloride concentration. In section 416.0–437.5 m, there was an increasing trend. However, the concentration levels stabilised at the end of the investigation period.

The iron concentrations determined by ICP-AES (total Fe) and by spectrophotometry (Fe(+II) and Fe-tot) are compared in Figures 7-4 and 7-5. The total iron concentrations determined by ICP agree reasonably well with the results obtained by spectrophotometry.

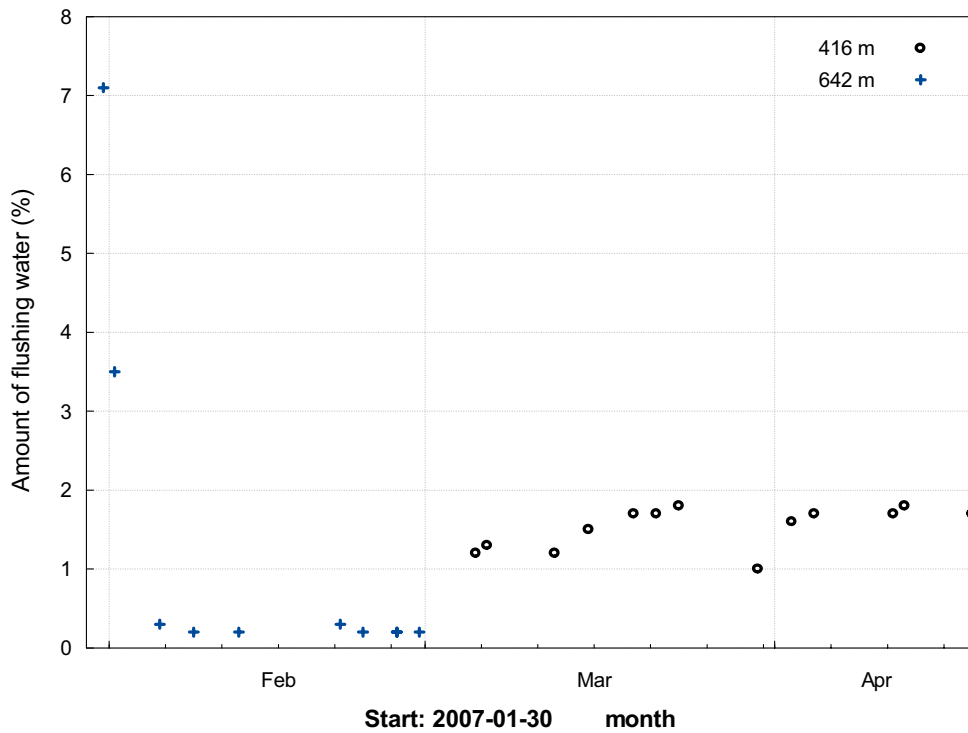


Figure 7-1. Flushing water content in the sample series collected during pumping in borehole sections 416.0–437.5 m and 642.0–701.1 m.

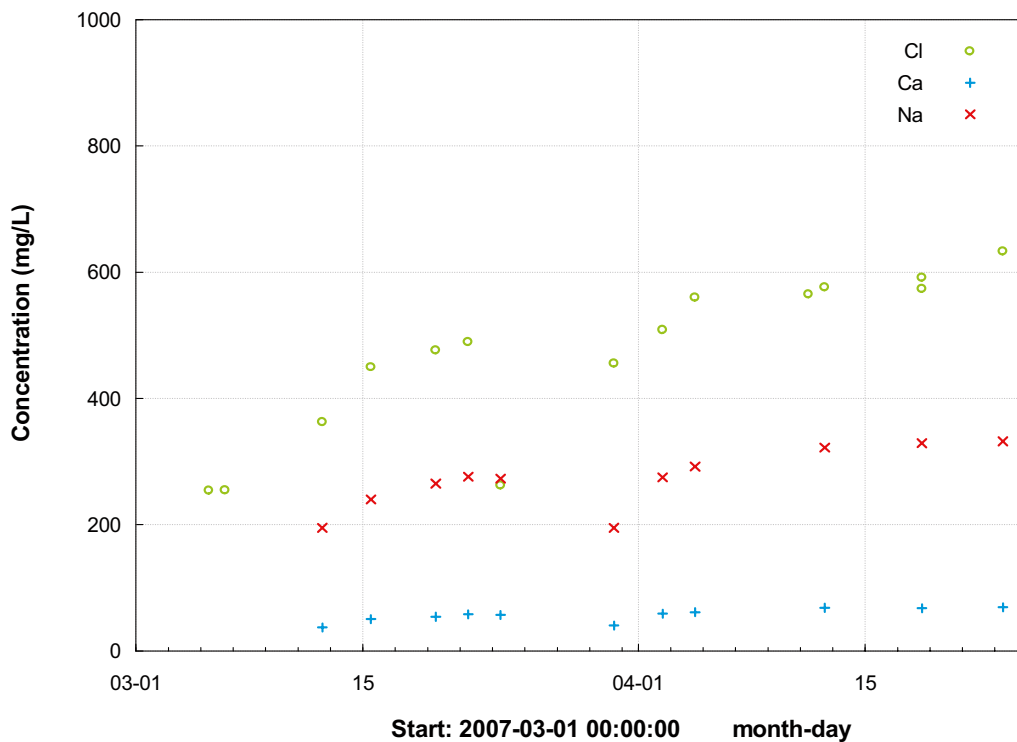


Figure 7-2. Chloride, calcium and sodium concentrations from sample series at 416.0–437.5 m.

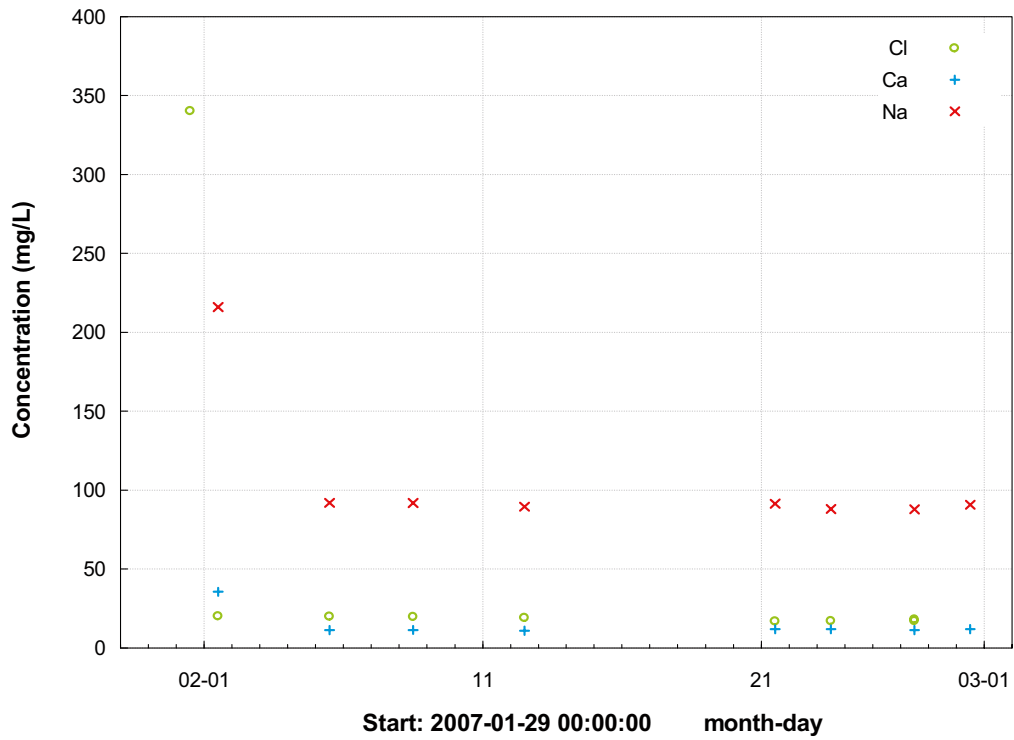


Figure 7-3. Chloride, calcium and sodium concentrations from sample series at 642.0–701.1 m.

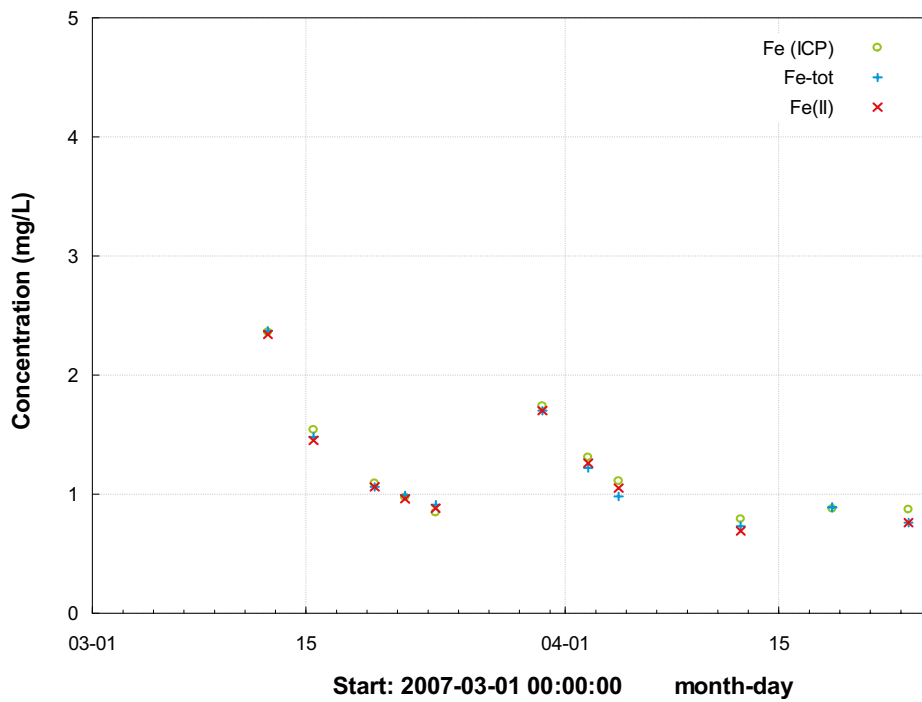


Figure 7-4. Comparison of iron concentrations obtained by ICP-AES and by spectrophotometry, borehole section 416.0–437.5 m.

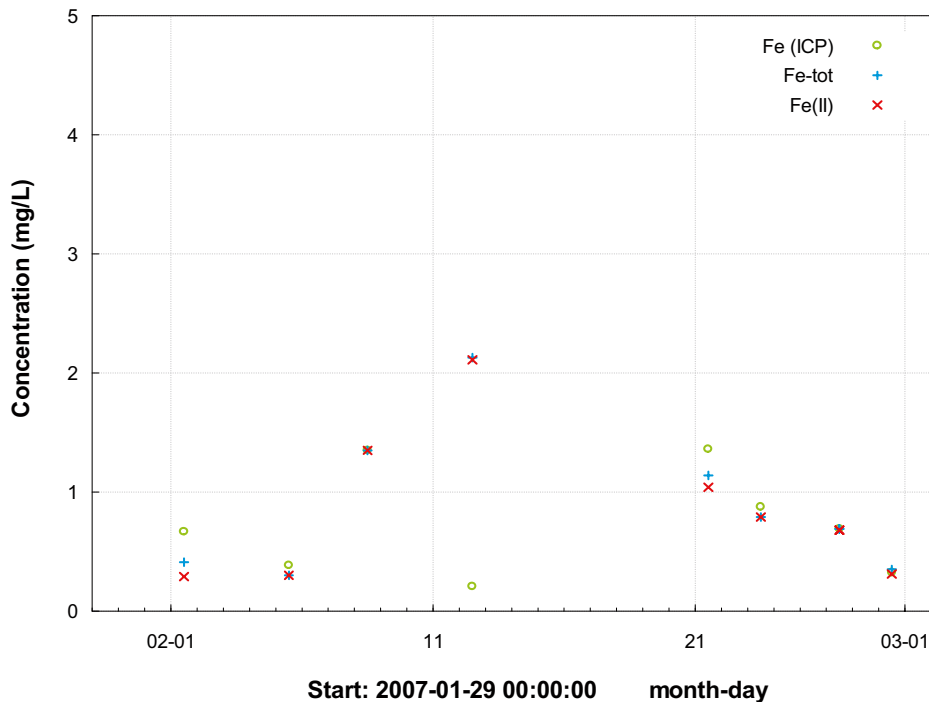


Figure 7-5. Comparison of iron concentrations obtained by ICP-AES and by spectrophotometry, borehole section 642.0–701.1 m.

Sulphate analysed by ion chromatography (IC) is compared with sulphate determined as total sulphur by ICP-AES in Figures 7-6 and 7-7. The sulphate concentrations remained constant in section 642.0–701.1 m, while in section 416.0–437.5 there was a slight increase in the concentration. The IC results are somewhat lower than the ICP results in all of the sections. Differences may be due to the presence of other sulphur species than sulphate, although experience has shown that ICP measurements may be more reliable since the variation between the samples in a time series often is smaller.

The chloride concentrations are plotted versus the corresponding electrical conductivity values in Figure 7-8. The plot gives a rough check of the data. As shown, the data from the borehole sections agree well with data obtained by earlier investigations from the Äspö Hard Rock Laboratory.

7.2.2 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 A10-2.

7.2.3 Stable and radioactive isotopes

The isotope determinations include the stable isotopes $\delta^2\text{H}$, $\delta^{18}\text{O}$, $^{10}\text{B}/^{11}\text{B}$, $\delta^{34}\text{S}$, $\delta^{13}\text{C}$ and $^{87}\text{Sr}/^{86}\text{Sr}$ as well as the radioactive isotopes ^3H (TU), ^{14}C (pmC), ^{238}U , ^{234}U , ^{230}Th , ^{226}Ra and ^{222}Rn . Isotope data are compiled in Appendix 10, Tables A10-3 and A10-4. The B-isotope ratio is given as $^{10}\text{B}/^{11}\text{B}$ (the result reported from the consulting laboratory). If one wants to use the notation according to international standard for environmental isotopes, $^{11}\text{B}/^{10}\text{B}$, it is necessary to invert the $^{10}\text{B}/^{11}\text{B}$ value ($1/^{10}\text{B}/^{11}\text{B}$).

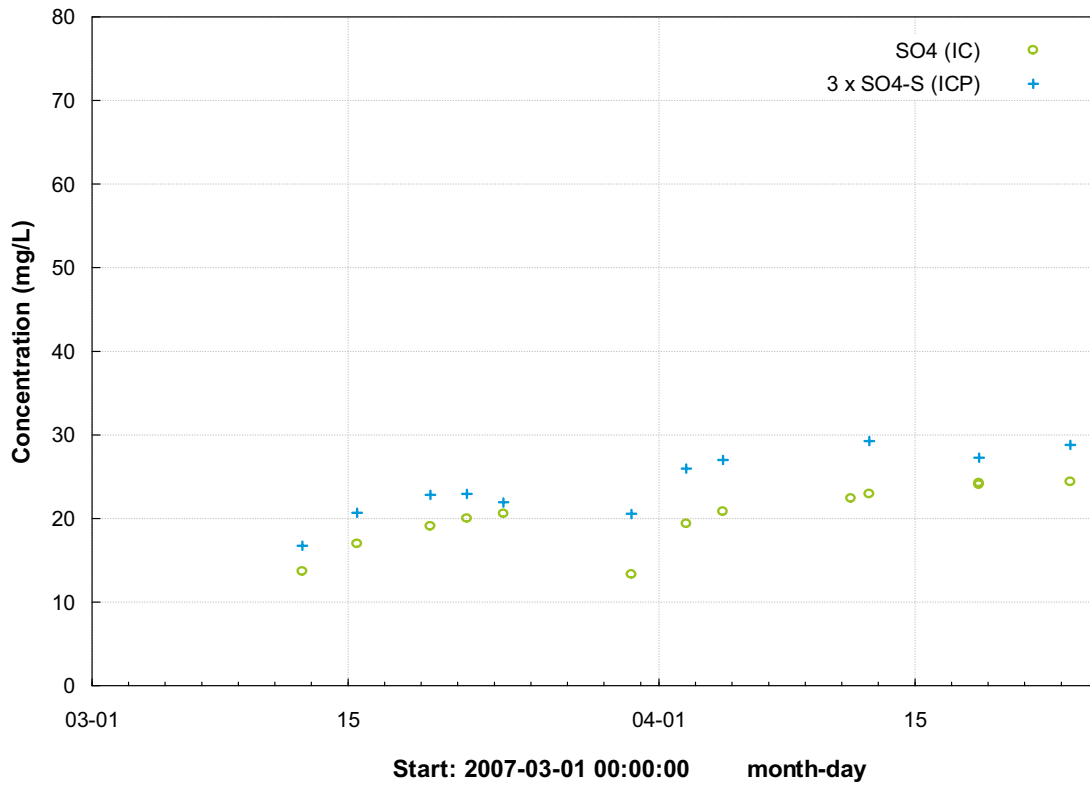


Figure 7-6. Sulphate (SO_4 by IC) to total sulphate calculated from total sulphur ($3 \times SO_4-S$ by ICP) versus date, borehole section 416.0–437.5 m.

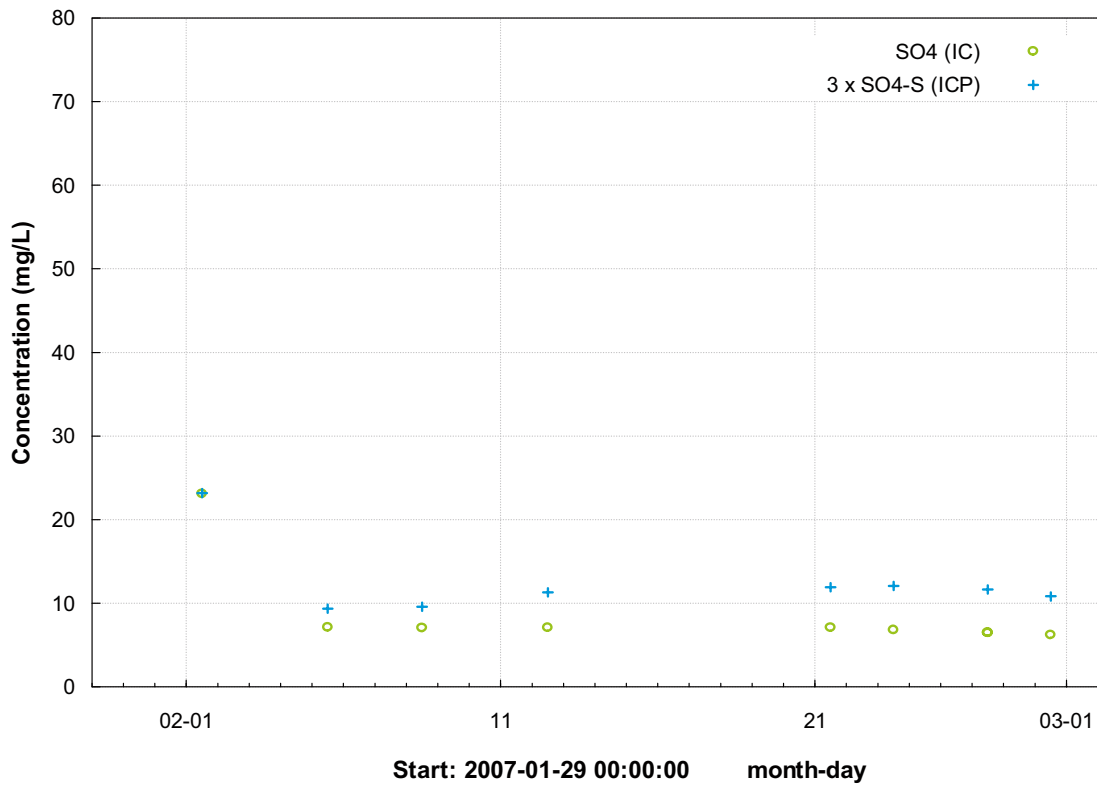


Figure 7-7. Sulphate (SO_4 by IC) to total sulphate calculated from total sulphur ($3 \times SO_4-S$ by ICP) versus date, borehole section 642.0–701.1 m.

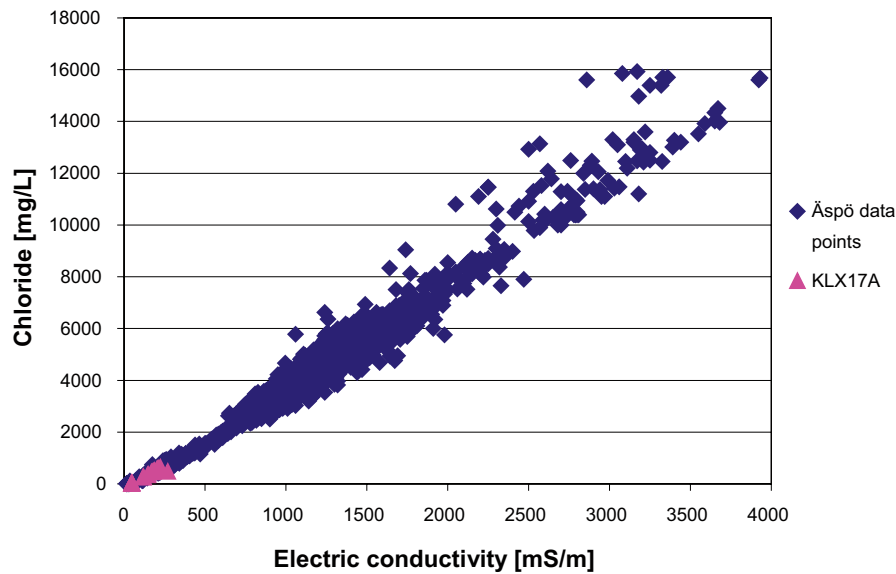


Figure 7-8. Chloride concentration versus electrical conductivity. Data from earlier investigations at the Äspö Hard Rock Laboratory are used to show the linear relationship. The data from KLX17A are consistent with previous investigations.

The ^3H and $\delta^{18}\text{O}$ results are presented in Figures 7-9 and 7-10. The $\delta^{18}\text{O}$ ratios remained stable during the end of the sampling periods. The ^3H content in both sections was above the detection limit (0.8 Tritium Units) in all samples except one. For section 642.0–701.1 m it cannot be excluded that a small leakage in the borehole pump has occurred (due to worn o-rings), resulting in contamination from deionised water¹ from the hydraulic pumping system. The enhanced ^3H concentration (32.2 ± 2.3 TU) in sample 11689 (2007-02-12) is most likely a consequence from a leakage in the borehole pump. The water tank to the driving water pump had to be refilled on the 13–14th of February. The ^3H containing deionised water in the hydraulic pumping system was replaced on the 26th of February before investigating section 416.0–437.5 m.

Since both sections are long (21 and 59 m respectively) it effects the turnover time for the water in the sections. Insufficient turnover of the water can possibly explain the ^3H and $\delta^{18}\text{O}$ concentrations in the beginning of the investigation sequences as well as for sample no 11770 (2007-03-30) and 11771 (2007-04-02) in section 416.0–437.5 m, which were preceded by lifting of the borehole equipment. However, at the current depth ^3H concentrations below detection limit would be expected. Leakage over the packers can not be excluded, although it is considered unlikely, since the packers were carefully placed where a minimum of fractures could be observed.

$\delta^{13}\text{C}$ and pmC were determined both in inorganic carbon (hydrogen carbonate) and in organic constituents. The results are presented in Table 7-2. Enrichment of organic carbon was necessary in order to collect enough organic material.

Table 7-2. Inorganic and organic $\delta^{13}\text{C}$ and pmC in water samples from KLX17A.

Borehole section (m)	Inorg. $\delta^{13}\text{C}$ (dev PDB)	Org. $\delta^{13}\text{C}$ (dev PDB)	Inorg. pmC	Org. pmC
416.0–437.5	-16.2	-26.8	41.0	71.0
642.0–701.1	-16.4	-	52.7	-

- not analysed

¹ Deionised water in the hydraulic pumping system might contain ^3H , SKB P-07-164.

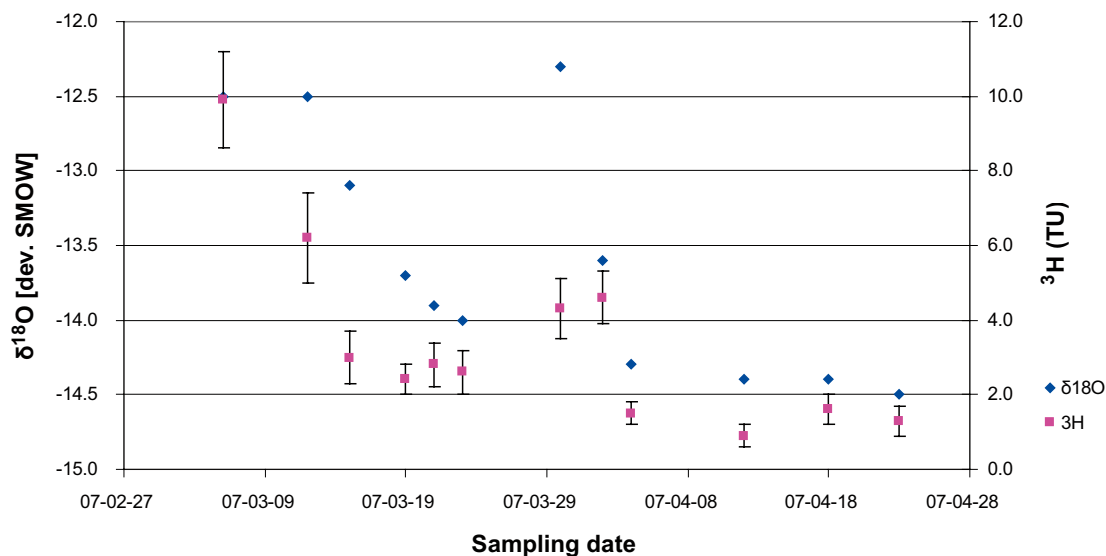


Figure 7-9. ³H and δ¹⁸O (‰ SMOW) data versus sampling date, section 416.0–437.5 m.

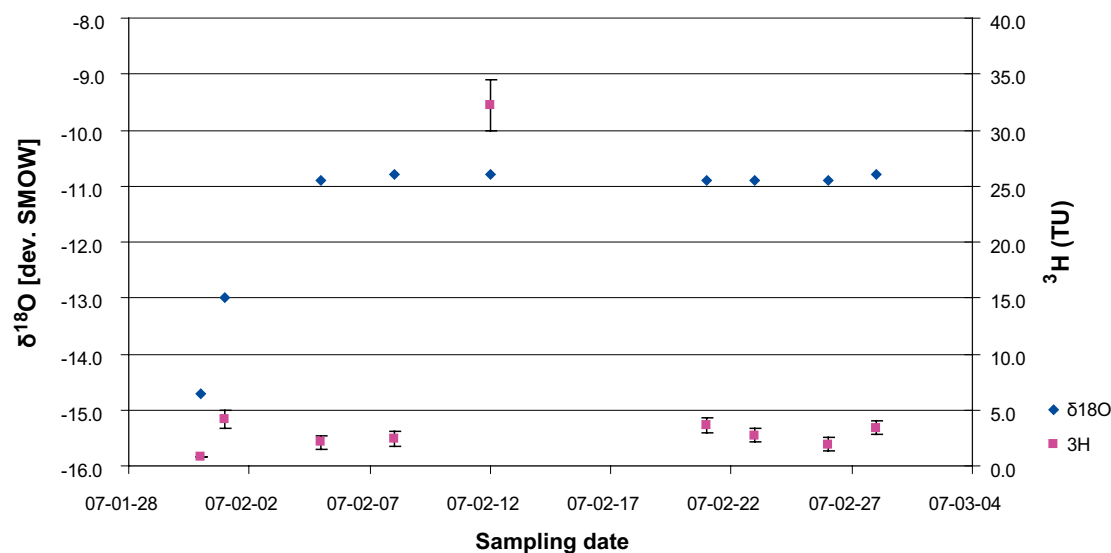


Figure 7-10. ³H and δ¹⁸O (‰ SMOW) data versus sampling date, section 642.0–701.1 m.

7.3 Dissolved gas

Sampling for gas was performed in sections 416.0–437.5 m and 642.0–701.1 m. Two containers with gas samples from each section were sent to two different laboratories (laboratory 1 and 2). Nitrogen gas was used for purging the samples. The analyses of dissolved gases include argon (Ar), helium (He), nitrogen (N₂), carbon dioxide (CO₂), carbon monoxide (CO), methane (CH₄), oxygen (O₂), hydrogen (H₂), ethane (C₂H₆), ethene (C₂H₄), ethyne (C₂H₂), propane (C₃H₈) and propene (C₃H₆). 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 7-3. The oxygen content indicates air leakage into the purging system at the consulted laboratory. The effects of air leakage may be corrected for, assuming that the oxygen content is zero, by removing the air effect (nitrogen, oxygen and argon).

Table 7-3. Total content of dissolved gas.

	Section 416.0–437.5 m		Section 642.0–701.1 m	
	Laboratory 1	Laboratory 2	Laboratory 1	Laboratory 2
Total gas content [mL/L]	67	120.6	237	66.4
Oxygen content [mL/L]	0.028	0.187	0.12	0

Both the total gas content and the concentrations of gases differed between the two samples in both sections. Probable reasons for the differences in concentrations are errors in analyses, incomplete purging of gas from the containers and contamination of air while purging.

The gas containers are pressurised with nitrogen gas (about 5 bar) during sampling. The volume percent nitrogen gas is comparable for both laboratories, which means that there is no effect of nitrogen gas on the total gas content. However, there is a relation between the gas content and the place of the container in the borehole; the container where the water enters first has the highest gas content. A plot between the vertical depth and the total gas content for several boreholes in the Oskarshamn investigation area suggest gas content > 50 and < 100 ml/liter water. Based on this information the representative gas concentrations are considered those reported by laboratory 1 in section 416.0–437.5 m (67 ml gas/liter) and laboratory 2 in section 642.0–701.1 m (66.4 ml gas/liter).

The gas compositions (in vol-%) of the samples from sections 416.0–437.5 m and 642.0–701.1 m are compared in Figure 7-11 and 7-12.

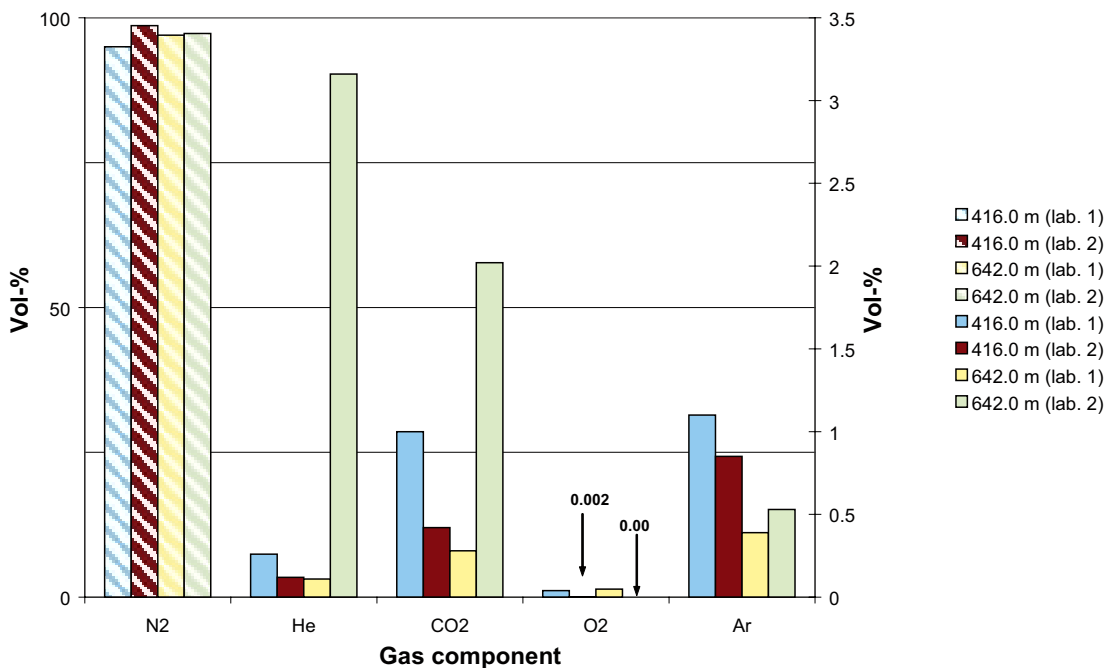


Figure 7-11. Gas components of high concentrations (N_2 , He, CO_2 , O_2 , Ar and CH_4) in samples collected in KLX17A using the in situ sampling equipment. Striped and non-striped bars refer to the scales on left and right axis, respectively.

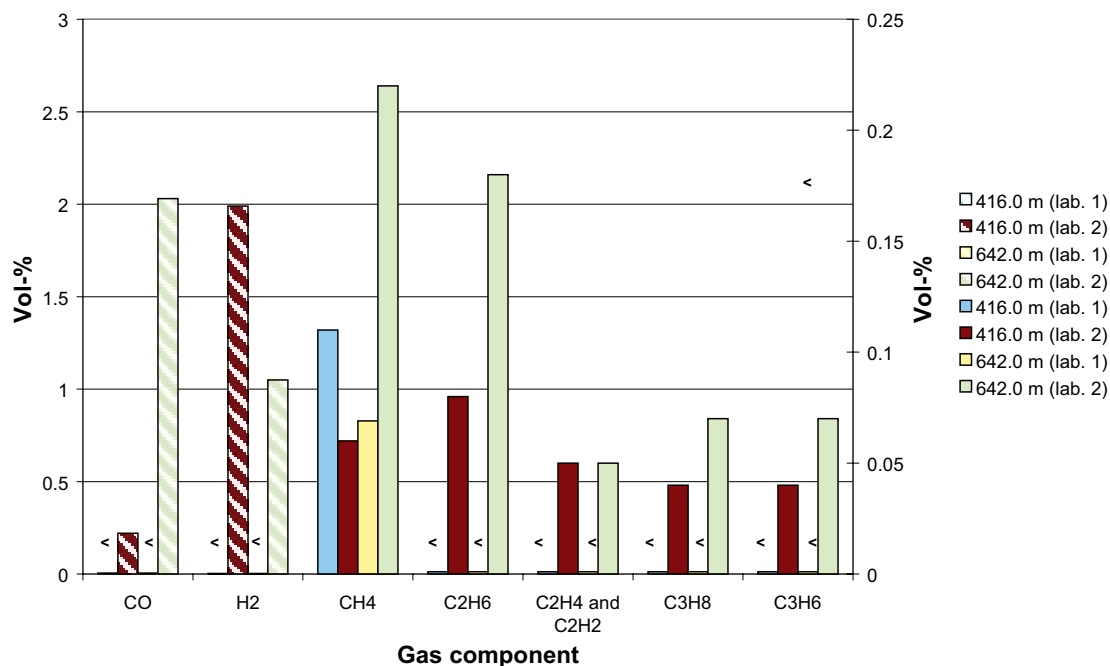


Figure 7-12. Gas components of low concentrations (CH_4 , CO , H_2 , C_2H_6 , sum of C_2H_4 and C_2H_2 , C_3H_8 and C_3H_6) in samples collected in KLX17A using the in situ sampling equipment. Striped and non-striped bars refer to the scales on left and right axis, respectively.

7.4 Colloids

The presence of colloids was investigated using three methods, 1) filtration through a series of connected filters in an argon atmosphere (two variations; detection by ICP-MS, “Filtration – ICP” (section 642.0–701.1 m) and by SEM, “Filtration – SEM” (reference 7; section 416.0–437.5 m), 2) fractionation/ultra filtration using two cylindrical filters with cut-offs of 1,000 D and 5,000 D and 3) Laser-Induced Breakdown Detection, LIBD, Appendix 8.

The results from the two methods 1) and 2) are difficult to compare quantitatively but a qualitative agreement is identified. However method 1) and 3) can be compared and the results from “Filtration – ICP”, “Filtration – SEM” and the LIBD determinations are presented in Table 7-4. The results from the filtration runs are corrected by considering the remaining water volume in each filter (indicated by the sodium content) and excluding its amounts of the different dissolved elements. Furthermore, the analysed elements are re-calculated to amounts of their most probable mineral phases (illite, iron hydroxide and manganese hydroxide).

An overview of colloid concentrations determined by LIBD in groundwater samples from boreholes at the Forsmark site investigation; KFM06A, KFM07A, KFM08A, and KFM01D, has been presented previously /8/.

There are some difficulties associated with colloid determinations. Generally, it is expected that the measured colloid concentrations turn out higher than the natural amount of background colloids in the groundwater as additional colloids are easily generated by artefacts. The sources may be:

- Oxygen intrusion and formation of iron hydroxide.
- Decrease of pressure and precipitation of calcite.
- The sampling process or the equipment.

Table 7-4. Colloid concentrations measured in the groundwater samples. Comparison of results obtained by “Filtration – ICP”, “Filtration – SEM” and LIBD.

Filtration through series of connected filters						LIBD/SEM		
Idcode/ secup/ filter pore size (µm)	Filtrate volume (mL)	Element content on each filter per litre of water (µg/L)				Mineral phases (µg/L) Sum**/ three filters	Idcode/ secup/ run no.	Content (µg/L)
		Al	Fe	Mn	Total/ filter*			
KLX17A/ 416.0/0.05 and 0.2	108.5						KLX17A/ 416.0/1	240/96
							KLX17A/ 416.0/2	110
KLX17A/ 642.0/0.2	177.0	70.6	32.4	0.091	103		KLX17A/ 642.0/1	Too high to report
KLX17A/ 642.0/0.05	177.0	13.6	35.2	0	48.9			
KLX17A/ 642.0/0.05	177.0	1.40	11.9	0.091	13.4	165	KLX17A/ 642.0/2	Too high to report

* Total content on each filter. Aluminium is calculated as 2.3 Al in K- Mg-illite (383.9 g/mol), iron is calculated as Fe(OH)₃ (106.8 g/mol) and manganese is calculated as Mn(OH)₂ (88.9 g/mol). The silicon, calcium and sulphur contents on the filters were below detection limit.

** Sum of content (mineral phases) on the three filters.

The colloid content in section 416.0–437.5 m is rather high, according to the LIBD determination as well as the SEM determination. In section 642.0–701.1 m it is too high to determine by the LIBD technique, although the result showing colloids containing aluminium and iron (analysed by SEM) is consistent with the ICP-MS results from the colloid filtration in section 642.0–701.1 m, but there is a discrepancy in the silicon analyses, see below.

7.4.1 Inorganic colloids – colloid filtration

In section 416.0–437.5 m colloid filtration was performed with a few changes and additions, as the colloid content was investigated using SEM /7/. A comparison with the SEM-analyses performed in connection with the LIBD determination (Appendix 8) can be made. In the SEM study the colloid morphology indicates a predominance of clay particles and the LIBD study shows that larger particles (several µm) consist of Si, Fe, Ca and Al / Si, thus the results are consistent.

The results from the colloid filtration performed in section 642.0–701.1 m are presented in Figures 7-13 to 7-18.

The bars in the diagrams represent amounts (µg) of aluminium, iron, silicon, manganese, sulphur and calcium entering the filter package, collected 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.

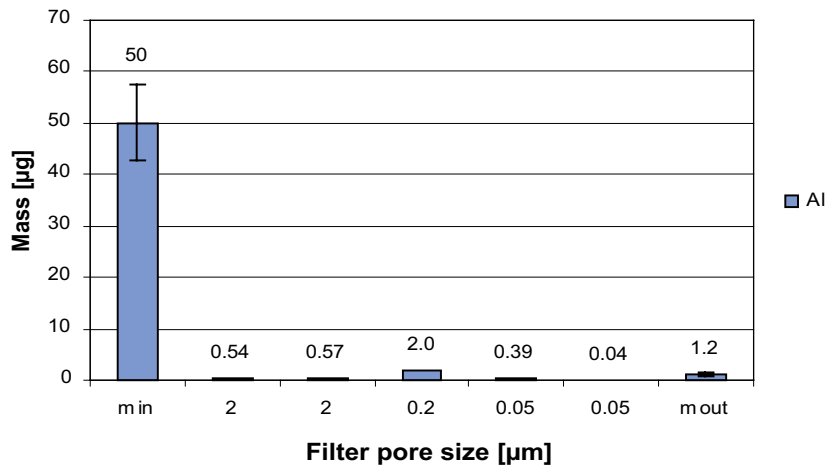


Figure 7-13. Amount of aluminium entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

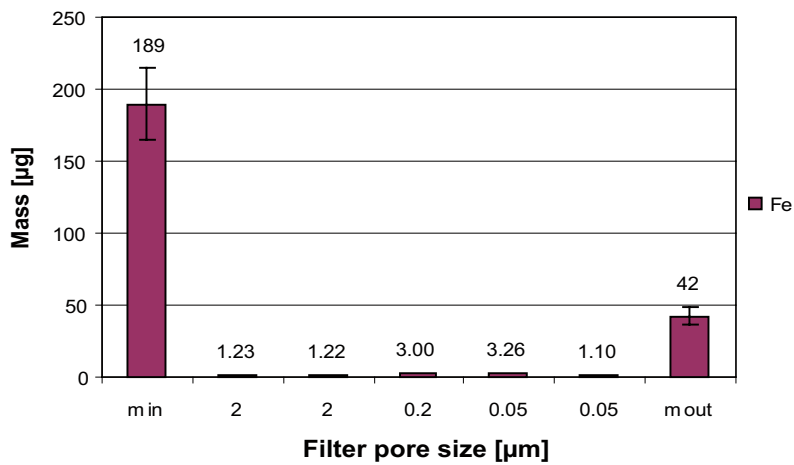


Figure 7-14. Amount of iron entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

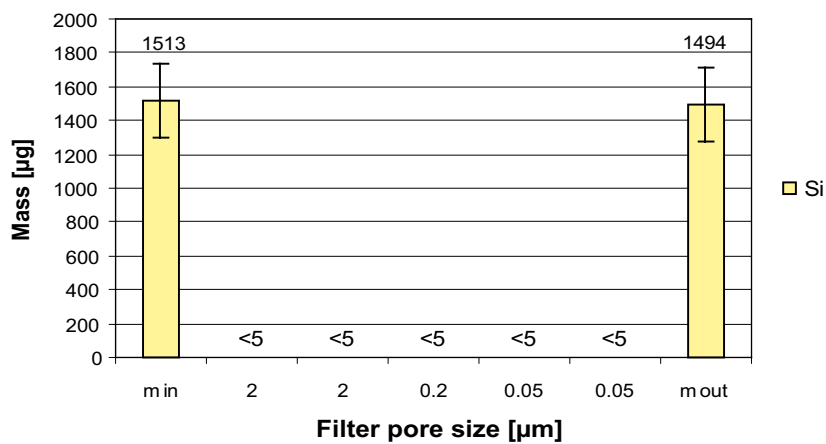


Figure 7-15. Amount of silicon entering the filter system (*m in*), in the filters and in the collecting container (*m out*).

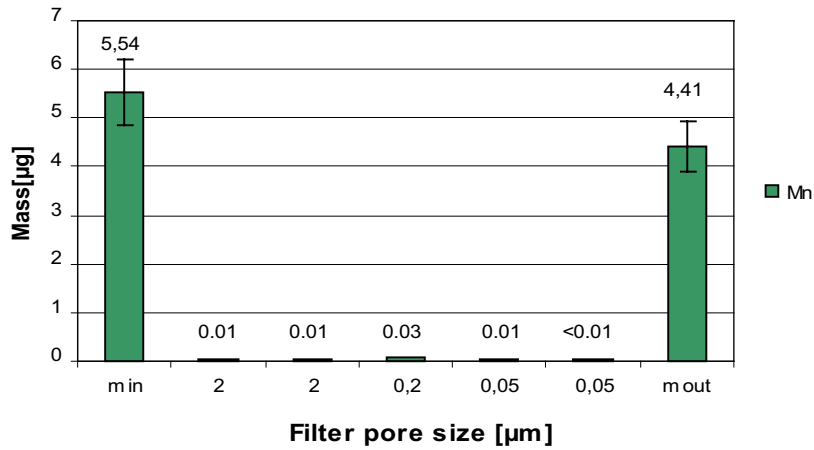


Figure 7-16. Amount of manganese entering the filter system (m in), in the filters and in the collecting container (m out).

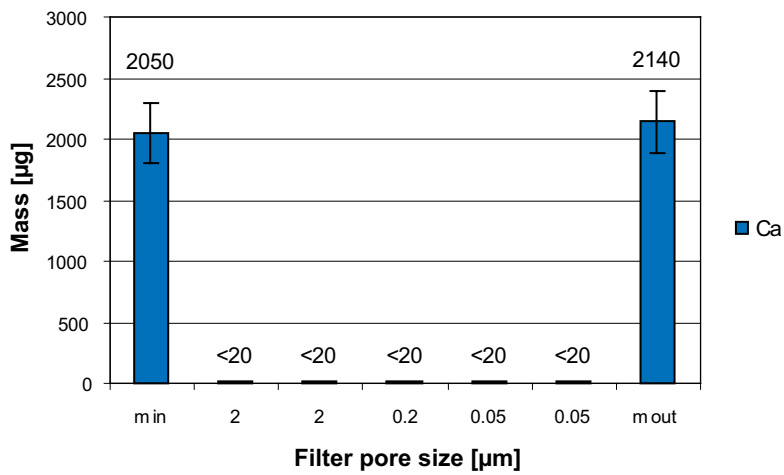


Figure 7-17. Amount of calcium entering the filter system (m in), in the filters and in the collecting container (m out).

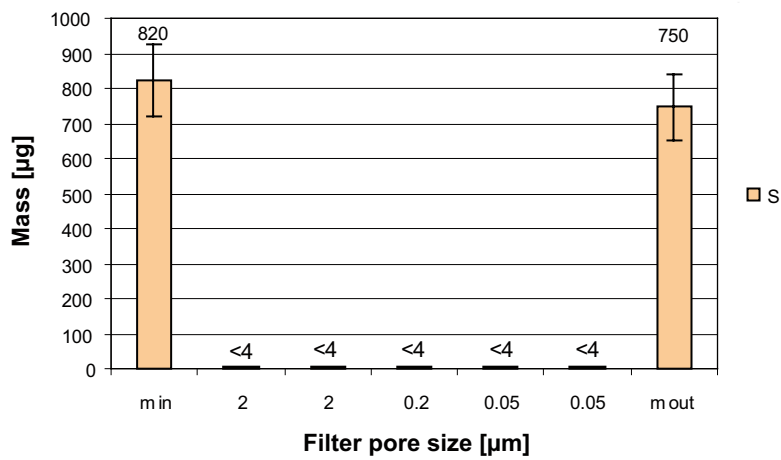


Figure 7-18. Amount of sulphur entering the filter system (m in), in the filters and in the collecting container (m out).

The concentrations in blank samples (rinsing water), PVB containers, collecting container and pumped groundwater are given in Table 7-5. The evaluation is complicated for iron and aluminium since precipitation and/or contamination have to be considered.

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

Both the iron and the aluminium concentration in the outgoing water is much lower than the amount detected in the collecting container after passing the filters despite that almost nothing is detected on the filters. This could be caused by precipitation of after passing the filtering system, possibly in the collecting container. Or, precipitation occurs in the PVB container which reduces the actual input concentration. Filter analyses of silicon and manganese as well as calcium and sulphur show values below the detection limits.

The following may be concluded from the colloid filtration results:

- The amounts present as colloidal iron and aluminium in sections 642.0–701.1 m are somewhat difficult to evaluate since the output amount plus the amount collected on filters does not balance the input amount. The reasons for this are contamination and/or precipitation in the PVB containers or in the collecting container.
- Low amounts of the investigated metals are detected on the filters. For silicon, calcium and sulphur the values are below the detection limit for all filters.
- The amount of silicon detected by SEM (in connection with the LIDB determination; Appendix 8) was higher than detected by ICP analysis of the filters. This is probably caused by insufficient leaching of the filters regarding silicon prior to the ICP analysis and it is possible that there are colloids containing silicon present in section 642.0–701.1 m.

7.4.2 Inorganic colloids-fractionation

Besides the DOC analyses, the samples from fractionation experiments were also analysed by ICP. 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.

Table 7-5. 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	Fe mg/L	Si mg/L	Mn µg/L	Ca mg/L	S mg/L
642.0–701.1	Blank, deionised water	1	0.011	<0.03	10.4	<0.2	<0.2
	Blank, leakage test	7	0.016	0.0679	15.6	0.111	<0.2
	Pumped water (alt. input conc.)	283	1.07	8.55	31.3	11.6	4.64
	Rest volume PVB (input conc.)	202 3,710	0.736 6.52	8.43 15.5	29.4 134	11.9 15.9	5.50 2.77
	Collecting container	7	0.24	8.44	24.9	12.1	4.22

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 Table 7-6 and Table 7-7 were calculated using mass balance equations. Silicon, aluminium, manganese, calcium and sulphur exist mainly 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. Small fractions of aluminium, manganese and sulphur with molecular weight more than 5,000 D were observed in section 642.0–701.1 m and a minor fraction of sulphur with molecular weight >5,000 D in section 416.0–437.5 m. .

The results for manganese, aluminium, iron in section 416.0–437.5 and iron in section 642.0–701.1 m are uncertain and omitted since precipitation or contamination might have occurred before or during filtering.

The blanks (de-ionised water collected after passing through the washed filters) showed insignificant concentrations of iron, silicon, calcium, aluminium, manganese, calcium and sulphur.

7.5 Humic and fulvic acids-fractionation

The results from fractionation of organic acids in sections 416.0–437.5 m and 642.0–701.1 m are summarised in Table 7-8. The water in section 416.0–437.5 m contains a fraction of organic acids with molecular weight less than 1,000 D as well as an equal fraction with molecular weight >1,000 D but < 5,000 D. The fractions consist of fulvic acids and possibly other low molecular weight organic acids such as citric acid and oxalic acids.

Table 7-6. Inorganic fractions (<1,000 D, 1,000 D to 5,000 D and >5,000 D) in section 416.0–437.5 m.

Fraction	Si [mg/L]	Ca [mg/L]	S [mg/L]
< 1,000 D	7.6 ± 1.1	51.9 ± 6.2	5.7 ± 0.7
< 5,000 D	7.9 ± 1.1	55.1 ± 6.1	6.8 ± 0.9
> 1,000 D but < 5,000 D	–	–	–
> 5,000 D	–	–	0.6 ± 0.2
Adsorption 1,000 D	–	–	–
Adsorption 5,000 D	–	–	–

Table 7-7. Inorganic fractions (<1,000 D, 1,000 D to 5,000 D and >5,000 D) in section 642.0–701.1 m.

Fraction	Si [mg/L]	Al [µg/L]	Mn [µg/L]	Ca [mg/L]	S [mg/L]
< 1,000 D	7.2 ± 1.1	3.2 ± 0.8	22.6 ± 2.8	10.1 ± 1.2	2.3 ± 0.3
< 5,000 D	7.1 ± 1.0	3.1 ± 0.9	22.8 ± 2.8	10.9 ± 1.3	2.6 ± 0.3
> 1,000 D but < 5,000 D	–	1.0 ± 0.3	–	–	–
> 5,000 D	–	1.3 ± 0.3	1.2 ± 0.7	–	0.2 ± 0.1
Adsorption 1,000 D	–	–	–	–	1.0 ± 0.6
Adsorption 5,000 D	–	–	–	–	0.9 ± 0.6

– = Below detection limit.

The results from the 1,000 D filter in section 642.0–701.1 m were not reliable. The concentration of organic carbon in the permeate was higher than the concentration of organic carbon in the borehole water. Contamination from the filter is unlikely since the sample blank contained organic carbon less than 1 mg/l. Possibly contamination from the vessel used for sampling the permeate might have occurred. The results for the 5,000 D filter suggest mainly a fraction of organic acids with molecular weight less than 5,000 D for section 642.0–701.1 m.

Table 7-8. Summary of fractionation results in KLX17A.

Section Fraction	416.0–437.5 m DOC [mg/L]	642.0–701.1 m DOC [mg/L]
< 1,000 D	1.8 ± 0.2	*
< 5,000 D	3.5 ± 0.5	4.5 ± 0.6
> 1,000 D but < 5,000 D	1.6 ± 0.2	*
> 5,000 D	–	0.9 ± 0.2
Adsorption 1,000 D	–	*
Adsorption 5,000 D	–	–

– = Below detection limit

* = Unreliable results.

8 Summary

The *Complete chemical characterisation* in KLX17A 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 section 642.0–701.1 m (0.2%) but not in section 416.0–437.5 m (1.7%).
- The salinity concentrations and electrical conductivity indicate that two different water systems have been investigated; the chloride concentrations and electrical conductivity were about 18 mg/L and 50 mS/m in section 642.0–701.1 m and 590 mg/L and 210 mS/m in section 416.0–437.5 m.
- The salinity was stable during the pumping and sampling period in section 642.0–701.1 m, while in section 416.0–437.5 m a slight increasing concentration trend was recognised in the beginning of the investigation. A stable salinity indicates that no mixing occurred with water from other fracture systems with a different water composition.
- The total turnover for the water in sections 416.0–437.5 m and 642.0–701.1 m was 40 and 10 times, respectively, and thus the groundwater compositions can be considered as fairly representative for the water bearing fractures in the investigated sections.
- The magnitude of $\delta^{18}\text{O}$, pmC and salinity in section 416.0–437.5 m indicate mixing with glacial melt water. However, this is not supported by the high ^3H concentrations. Possible but unlikely explanations could be leakage over the packers or contamination from the hydraulic pumping system. The salinity in section 642.0–701.1 m was unusually low (18 mg/L), however, influence of fresh water from the surface is contradicted by the pmC signature. A likely explanation for the high ^3H concentrations in this section is contamination from the hydraulic pumping system.
- The quality of the water analyses is generally high, based on comparison between results from different laboratories, methods and acceptable charge balance errors. The relative errors are all within $\pm 5\%$, except for one sample (5.8%).
- The redox potential measurements from the electrodes in sections 416.0–437.5 m and 642.0–701.1 m appear to be of good quality. The electrodes (gold, glassy carbon and platinum) reached stable and consistent values; about -300 mV in both sections. Calculated redox potentials from the LIBD experiment are consistent with the on line measurements, while the measured potentials are 60–80 mV higher.
- The results from the colloid determination using LIBD in section 416.0–437.5 m show a rather high content of colloids. The mass concentration from the two analysed containers differed by a factor two. The colloid content determined by filtration - SEM shows agreement with the lower value and that there is a predominance of clay particles.
- In section 642.0–701.1 m, the colloid content was too high to determine by LIBD-technique, while the content according to the Filtration – ICP determination was 165 $\mu\text{g/L}$. The results from colloid Filtration - ICP and SEM in connection with the LIBD determination indicate that the contents of manganese, calcium and sulphur colloids in the groundwater are low or non-existent. The evaluation and comparison between the two methods is more complicated for iron and aluminium because of possible contamination and/or precipitation during filtration. However, the results from the SEM determination in connection with LIBD suggest that the colloid content is dominated by aluminium, silicon (alumino-silicates, silicates), fluoride and iron.
- The organic constituents are mainly present as fulvic acids and possibly other low molecular weight organic acids (citric and oxalic acids).

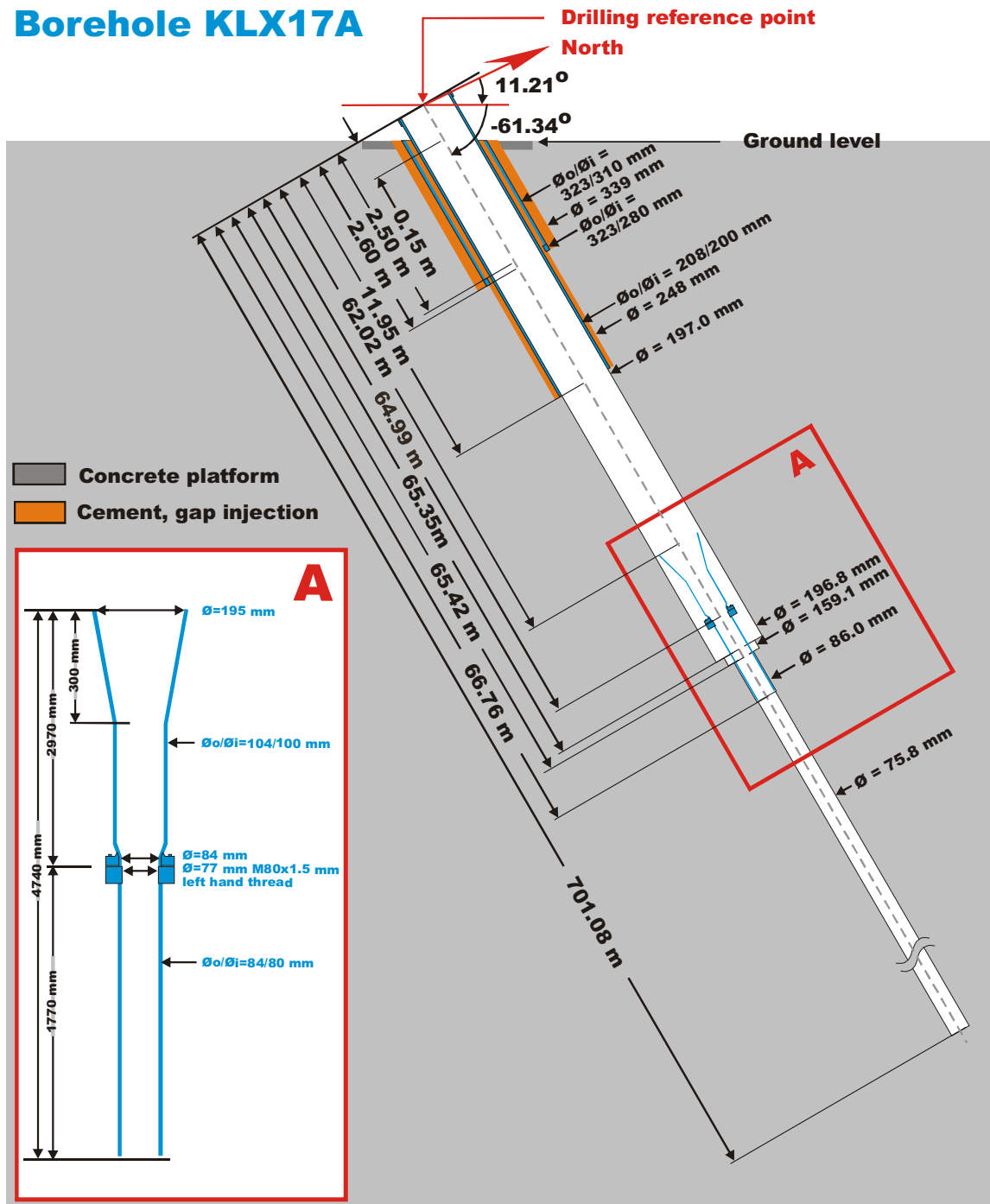
References

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- /2/ **Pedersen K, 2008.** Oskarshamn site investigation. Microorganisms in groundwater from boreholes KLX13A and KLX17A: numbers, viability, and metabolic diversity. Results from three sections: 432.0–439.2 m in KLX13A and 416.0–437.5 m and 642.0–701.1 m in KLX17A. SKB P-08-08 (in press), Svensk Kärnbränslehantering AB.
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- /5/ **Nielsen U T, Ringgaard J, 2006.** Oskarshamn site investigation. Geophysical borehole logging in boreholes KLX17A and HLX43. SKB P-06-315, Svensk Kärnbränslehantering AB.
- /6/ **Pöllänen J, Kristansson S, 2007.** Oskarshamn site investigation. Difference flow logging of borehole KLX17A. Subarea Laxemar. SKB P-07-34, Svensk Kärnbränslehantering AB.
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- /8/ **Nilsson K, Bergelin A, Lindqvist A, Nilsson A-C, 2006.** Forsmark site investigation. Hydrochemical characterisation in borehole KFM01D. Results from seven investigated borehole sections: 194.0–195.0 m, 263.8–364.8 m, 314.5–319.5 m, 354.9–355.9 m, 369.0–370.0 m, 428.5–435.6 m, 568.0–575.1 m. SKB P-06-227, Svensk Kärnbränslehantering AB.

Design of cored borehole KLX17A

Technical data

Borehole KLX17A



Drilling reference point

Northing: 6366848.75 (m), RT90 2,5 gon V 0:-15
Easting: 1546862.09 (m), RT90 2,5 gon V 0:-15
Elevation: 27.63 (m), RHB 70

Drilling period

Drilling start date: 2006-08-07
Drilling stop date: 2006-10-23

Results of difference flow logging in KLX17A

Laxemar, borehole KLX17A

Flow rate, caliper and single point resistance

- △ Without pumping (L=5 m, dL=5 m), (Flow direction = into the hole)
- ▽ Without pumping (L=5 m, dL=5 m), (Flow direction = into the bedrock)
- △ With pumping (Drawdown X m, L=5 m, dL=5 m), (Flow direction = into the hole)
- Without pumping (L=5 m, dL=0.5 m), 2006-12-10 - 2006-12-11
- With pumping (L=5 m, dL=0.5 m), 2006-12-13 - 2006-12-14
- With pumping (L=1 m, dL=0.1 m), 2007-01-04 - 2007-01-07
- With pumping during fracture-EC (L=0.5 m, dL=0.1 m), 2007-01-07 - 2007-01-08
- Lower limit of flow rate

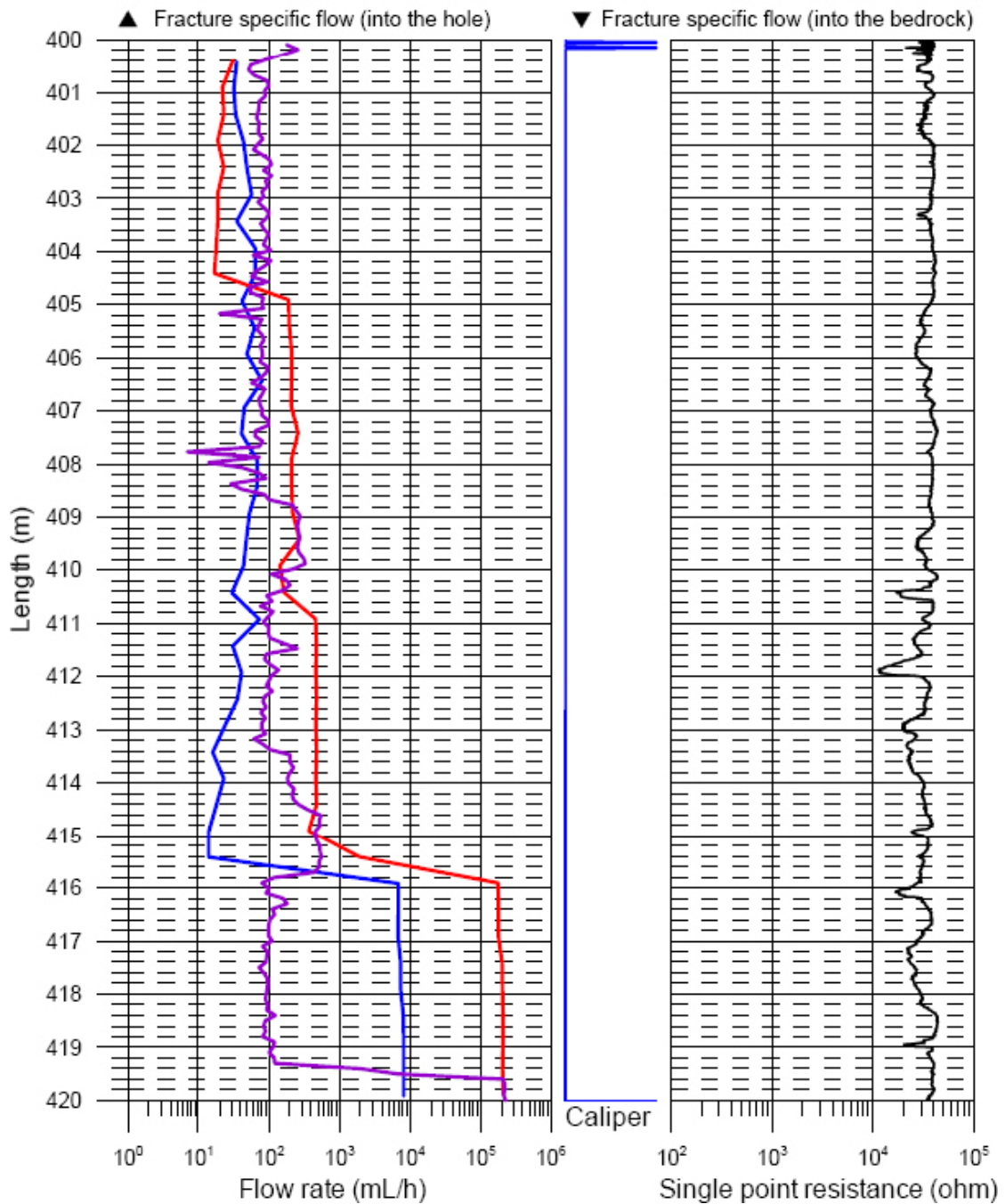


Figure A2-1a. Borehole KLX17A: Differential flow measurements from 400–420 m including the water bearing fracture zones at approximately 416–437 m /6/.

Laxemar, borehole KLX17A
Flow rate, caliper and single point resistance

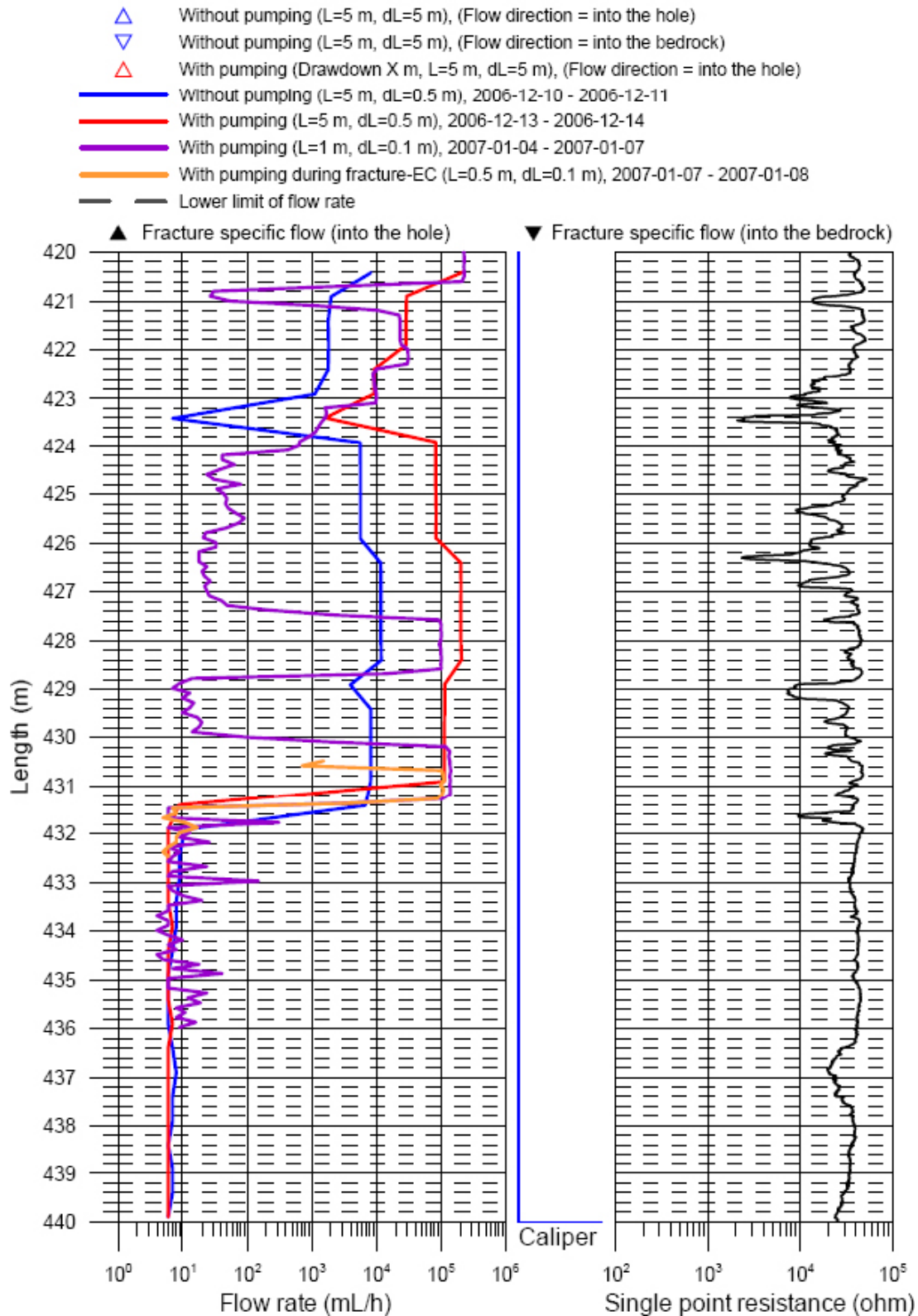


Figure A2-1b. Borehole KLX17A: Differential flow measurements from 420–440 m including the water bearing fracture zones at approximately 416–437 m /6/.

Laxemar, borehole KLX17A
 Flow rate, caliper and single point resistance

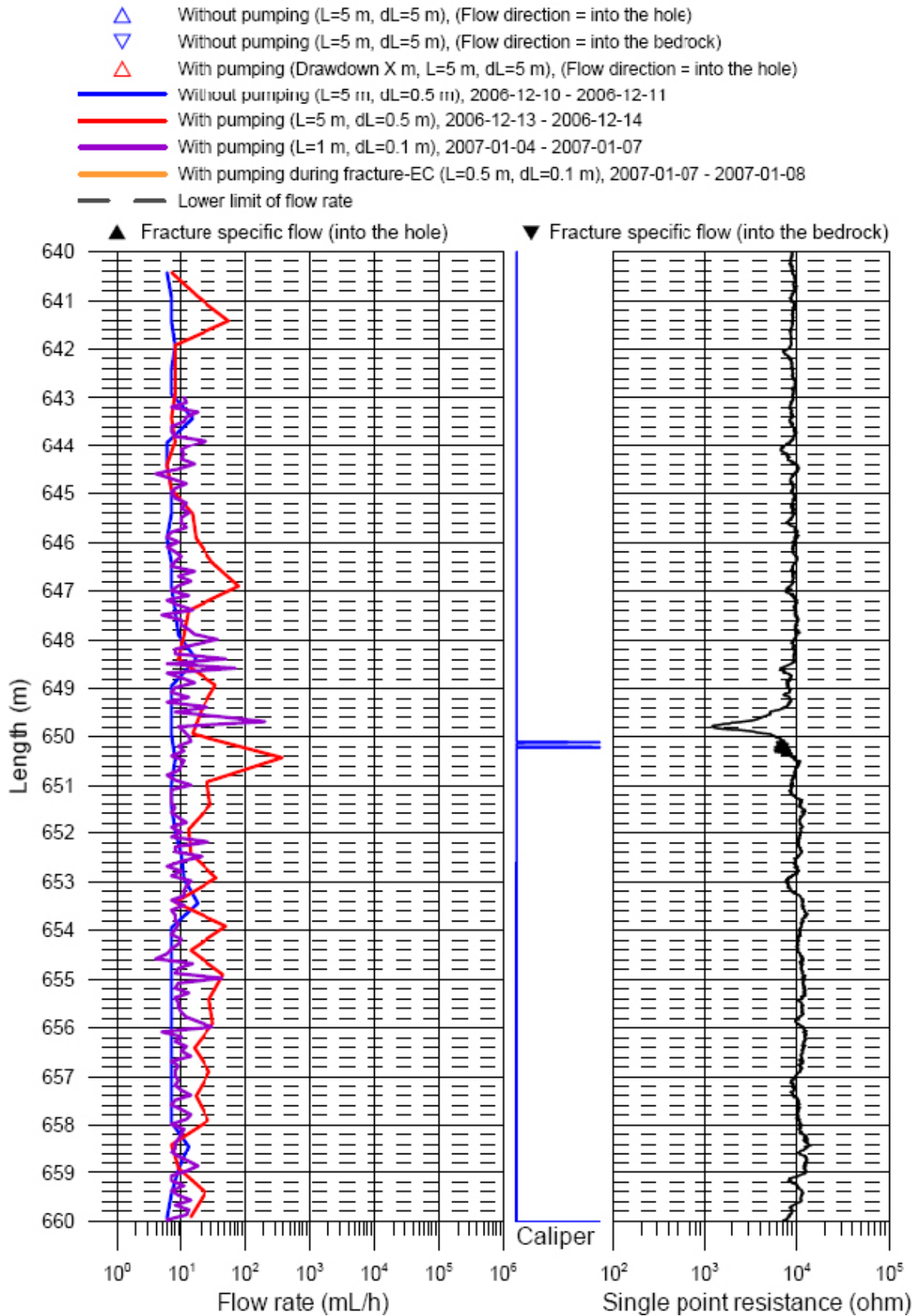


Figure A2-2a. Borehole KLX17A: Differential flow measurements from 640–660 m including the water bearing fracture zones at approximately 642–701 m /6/.

Laxemar, borehole KLX17A
 Flow rate, caliper and single point resistance

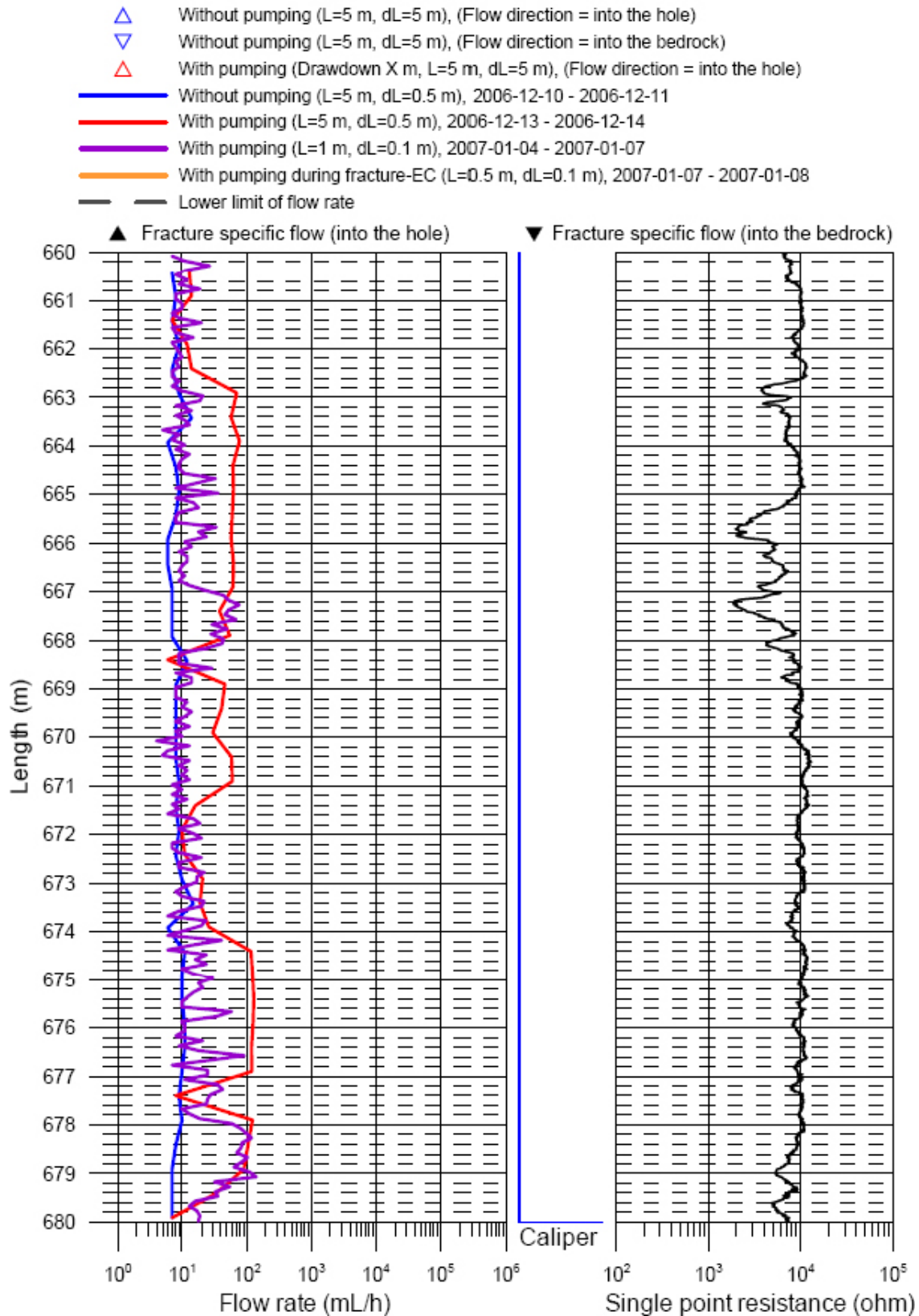


Figure A2-2b. Borehole KLX17A: Differential flow measurements from 660–680 m including the water bearing fracture zones at approximately 642–701 m /6/.

Laxemar, borehole KLX17A
 Flow rate, caliper and single point resistance

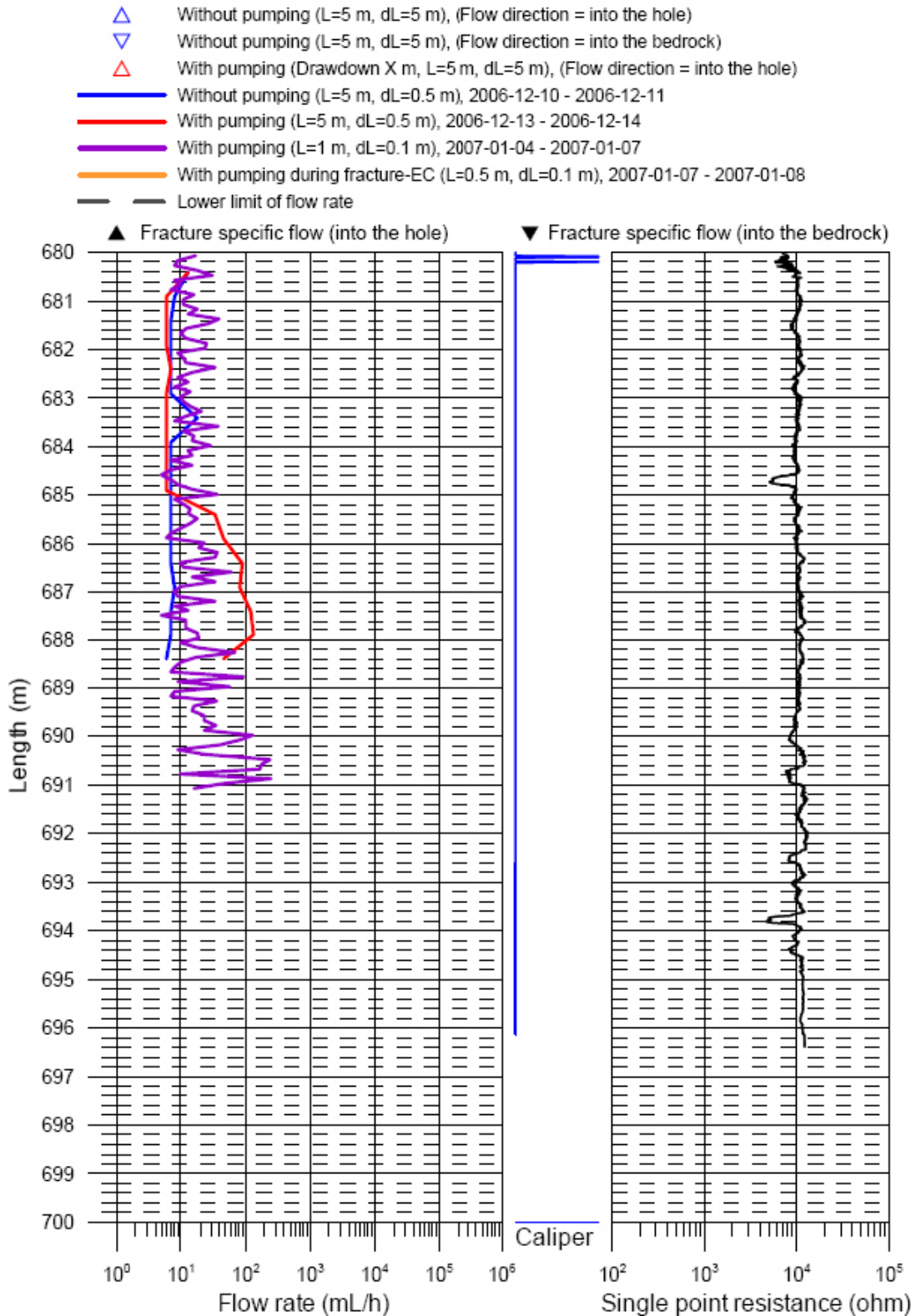


Figure A2-2c. Borehole KLX17A: Differential flow measurements from 680–700 m including the water bearing fracture zones at approximately 642–701 m /6/.

Selected images from BIPS logging in KLX17A

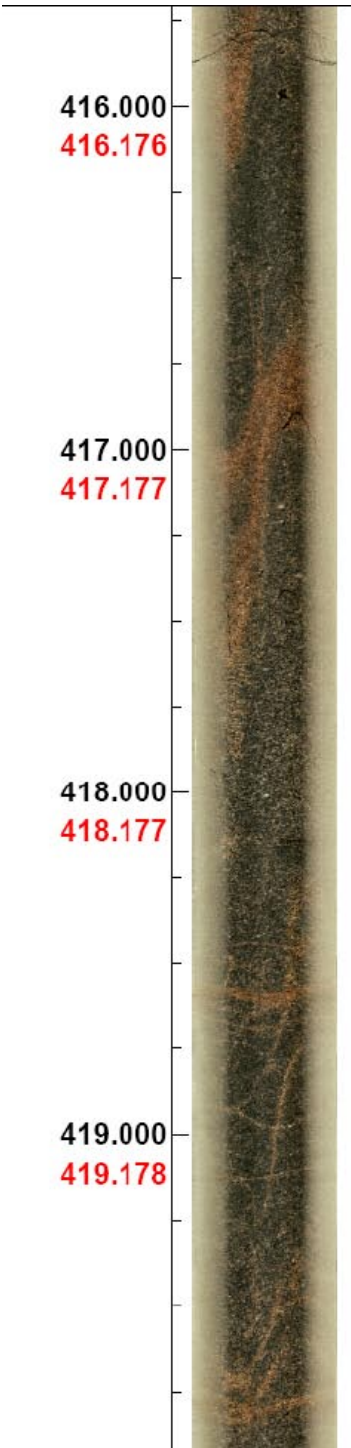


Figure A3-1a. Borehole KLX17A: selected BIPS logging image from 416.0 to 420.0 m including the water bearing fractures at 416–437 m. The non-adjusted length is marked with black and the adjusted true length is marked with red /4/.



Figure A3-1b. Borehole KLX17A: selected BIPS logging image from 420.0 to 440.0 m including the water bearing fractures at 416–437 m. The non-adjusted length is marked with black and the adjusted true length is marked with red /4/.

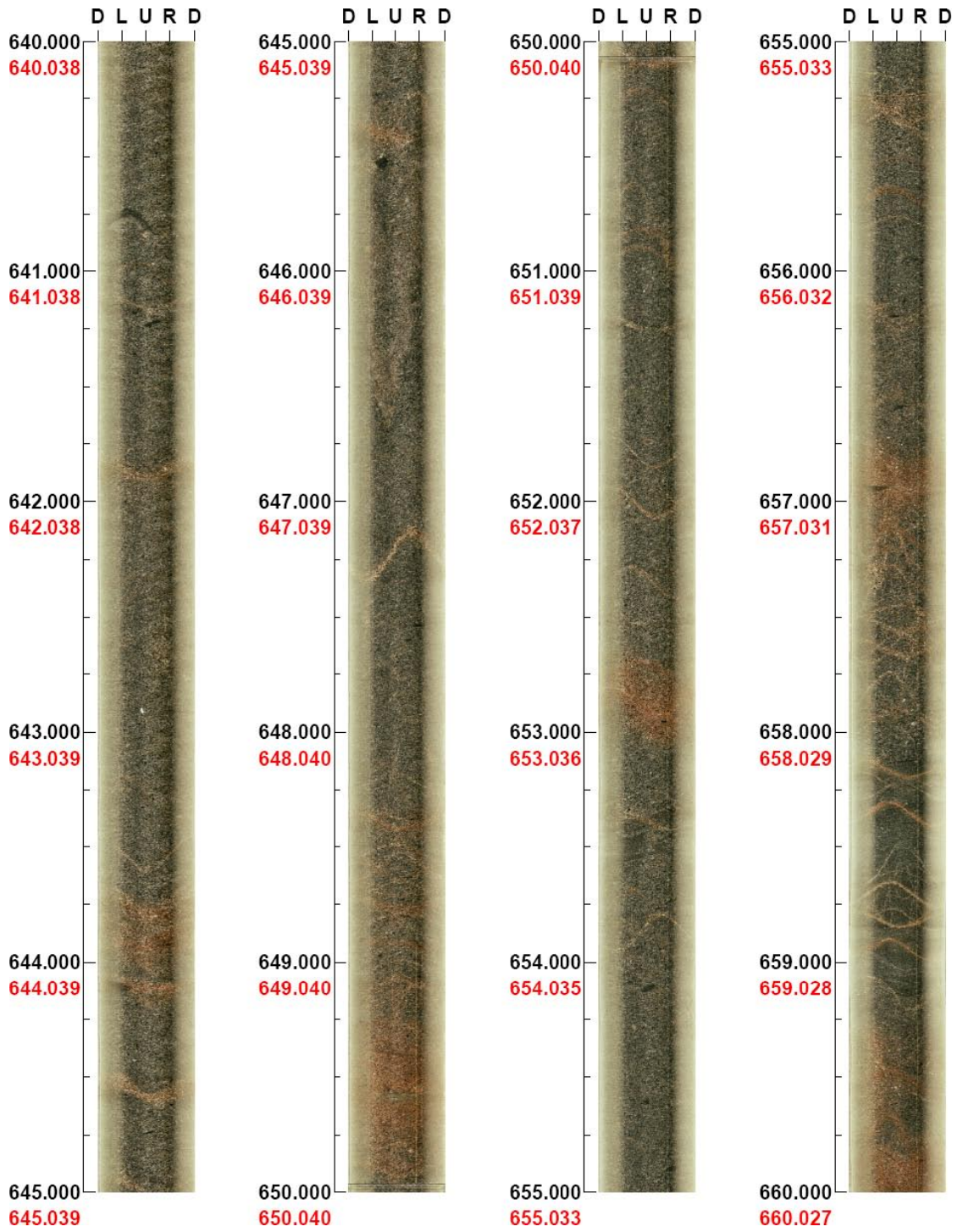


Figure A3-2a. Borehole KLX17A: selected BIPS logging image from 640 to 660 m including the water bearing fractures at 642–701 m. The non-adjusted length is marked with black and the adjusted true length is marked with red /4/.



Figure A3-2b. Borehole KLX17A: selected BIPS logging image from 660 to 680 m including the water bearing fractures at 642–701 m. The non-adjusted length is marked with black and the adjusted true length is marked with red /4/.

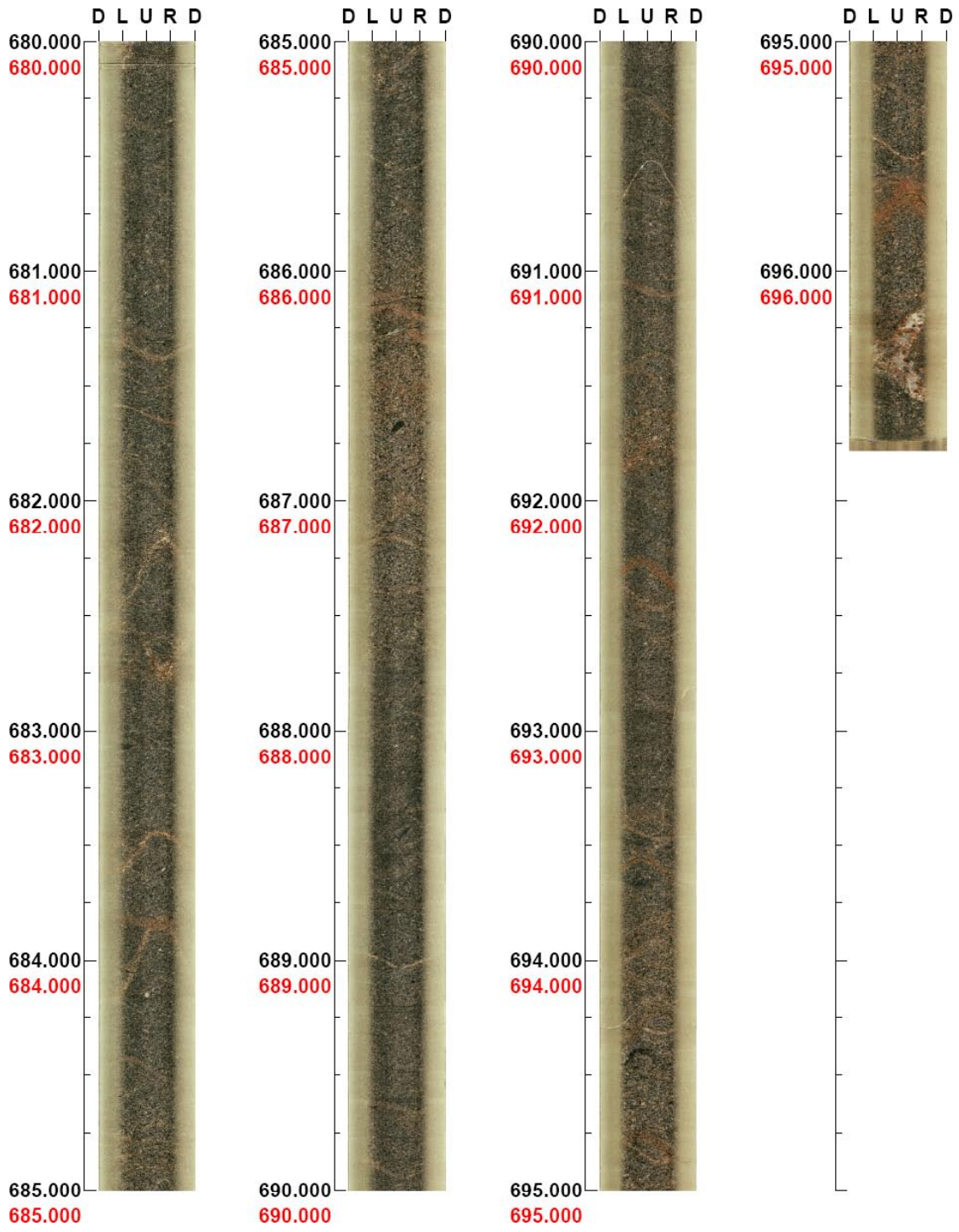


Figure A3-2c. Borehole KLX17A: selected BIPS logging image from 680 to 696 m including the water bearing fractures at 642–701 m. The non-adjusted length is marked with black and the adjusted true length is marked with red /4/.

Measurement information KLX17A

Section 416.0–437.5 m

Mätapplikation - SKB
File Special Development!

Mätapplikation Huvudmeny
MATDATOR1

Administration GivarKonf. B.Utr.Konf. Mätning Larm Logga Ut
System Kemkal. LängdKal. Trend Forcerad mät
Larmgränser Referenser GSM-larm HistLog Till kgn

Givarkonfiguration - S2 Vattenprovtagare Omgivning/Process

Borrhålschemac 2. 1. 3. 4. Temp Gnd

Ytchemmac 288 HRF 262 HRF 198 HRF 186 HRF 202 HRF 194 HRF 192 HRF 284 HRF 204 HRF 274 HRF -2 HRF -2 HRF -2 HRF -2 HRF tom tom 272 HRF 228 HRF

Ytchemmac, Id:	MYC2	Anm.	Typ	Id	Datum	Nod	Kanal
9.	EO2Y	40296	031023	4	17		
10.	EREG2Y	p9-3	040112	4	4		
11.	EREG1Y	P9-3	051102	3	4		
12.	EPHY	WD	031023	3	3		
13.	EPHY	WD	040419	3	6		
14.	EPHY	N9-1	031023	3	2		
15.	EAUY	P8-1	031023	3	1		
16.				0	0		
17.	ET1Y	Pt100	031023	4	15		
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		
	Q			4	9		
	V1Y			3	19		

Sond 2: 100000100111111
Sond 3: 1000000111101111
Sond 4: 100001100001000

Borrhålschemac, Id:Ke 021	Amn. Ja	Typ	Id	Datum	Nod	Kanal
Temp	ETB	M-FK 422	020911	2	15	156 HRF
1.	EPHD	G47	070301	2	1	128 HRF
2.	ECB	C2 96	041001	2	2	130 HRF
3.	EPHD	G40	070301	2	3	132 HRF
4.	EREGD	P37	070301	2	4	134 HRF
5.	EAUB	AU 021	020911	2	5	136 HRF
6.	EPTD	Pt 021	020911	2	6	138 HRF
Gnd				3	8	206 HRF
	PB	1682925	020202	2	9	144 HRF
	VI ARM			2	20	166 HRF
	VB			2	19	164 HRF

Figure A4-1. Electrode configuration, section 416.0–437.5 m.

Mätapplikation - SKB
File Special Development!

Mätapplikation Huvudmeny
MATDATOR1

Administration GivarKonf. B.Utr.Konf. Mätning Larm Logga Ut
System Kemkal. LängdKal. Trend Forcerad mät
Larmgränser Referenser GSM-larm HistLog Till kgn

Konfiguration av borrhålsutrustning

Typ av enhet	Id	Längd, mm	Avstånd mellan multikoppling och tätning	Dummy Id
Multislang	Multislang S2	1		
Spårdektör	SP022	1005		
Borrhålschemac	Kc 021	1245		
Ö. Manschett	Övre mans S2	2065	500	ingen
Hydr. Pump	Pump 022	2406		ingen
Vattenprovtagare	PVP 022	2505		ingen
Ex. Behållare	Fx 021	1475		
Förlängning	Rör 7 st	14235		
N. Manschett	Nedre MA S2	2065	390	ingen dummy

Total sondlängd: 27001, mm
Längd till Övre Manschett: 3815, mm
Längd till Nedre Manschett: 25326, mm
Sektionslängd: 21511, mm

Figure A4-2. Configuration of downhole equipment, section 416.0–437.5 m.

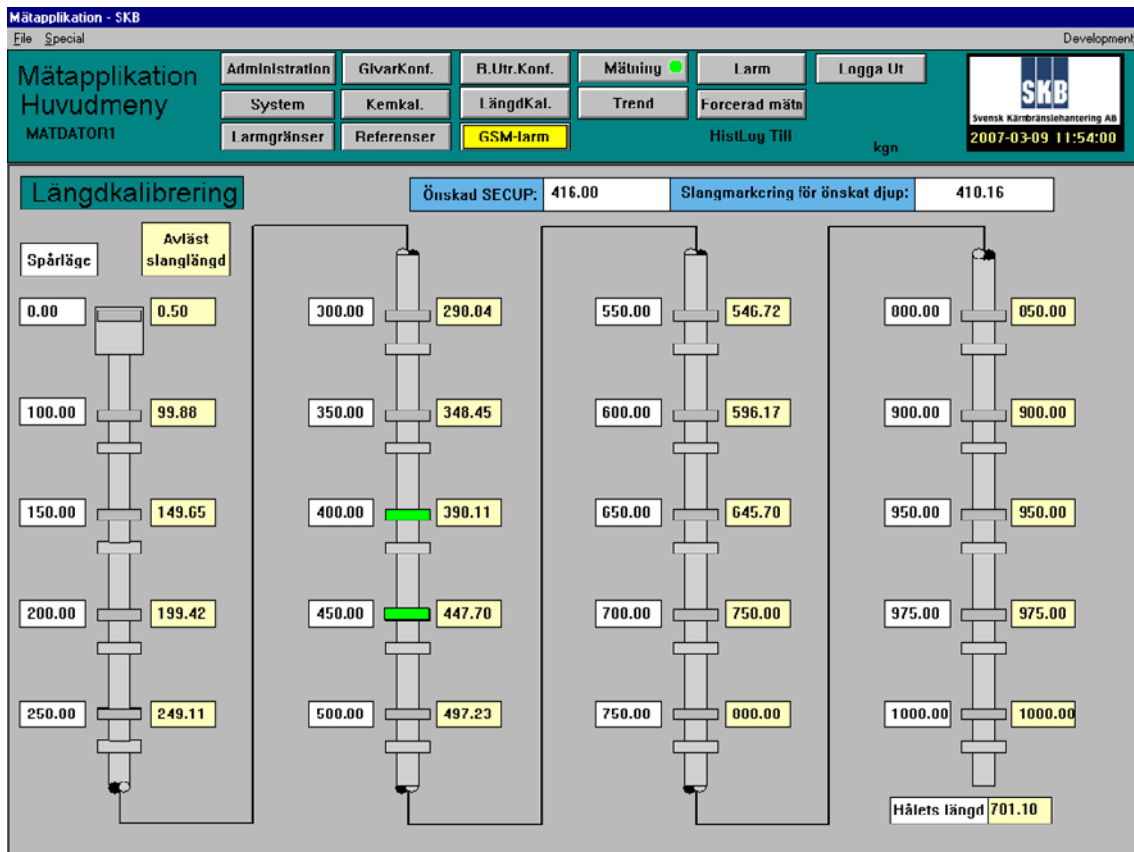


Figure A4-3. Length calibration, section 416.0–437.5 m.

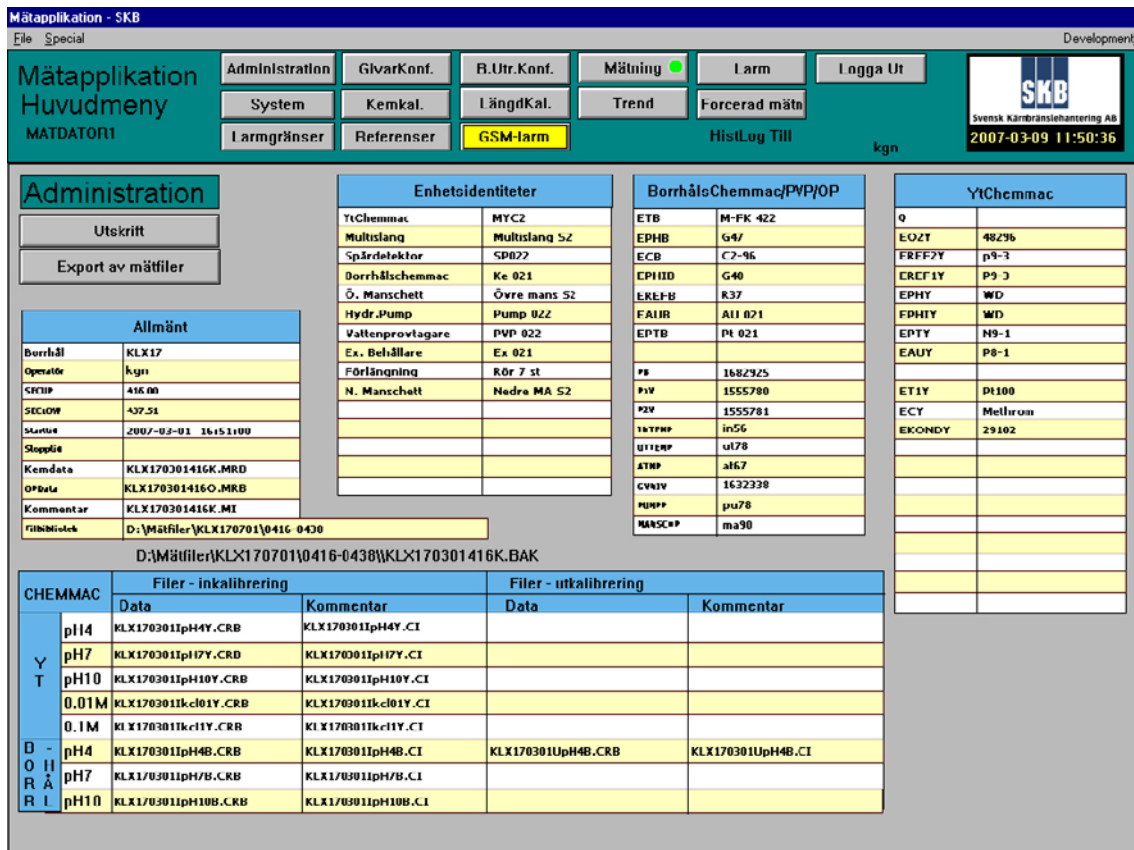


Figure A4-4. Administration, section 416.0–437.5 m.

Section 642.0–701.1 m

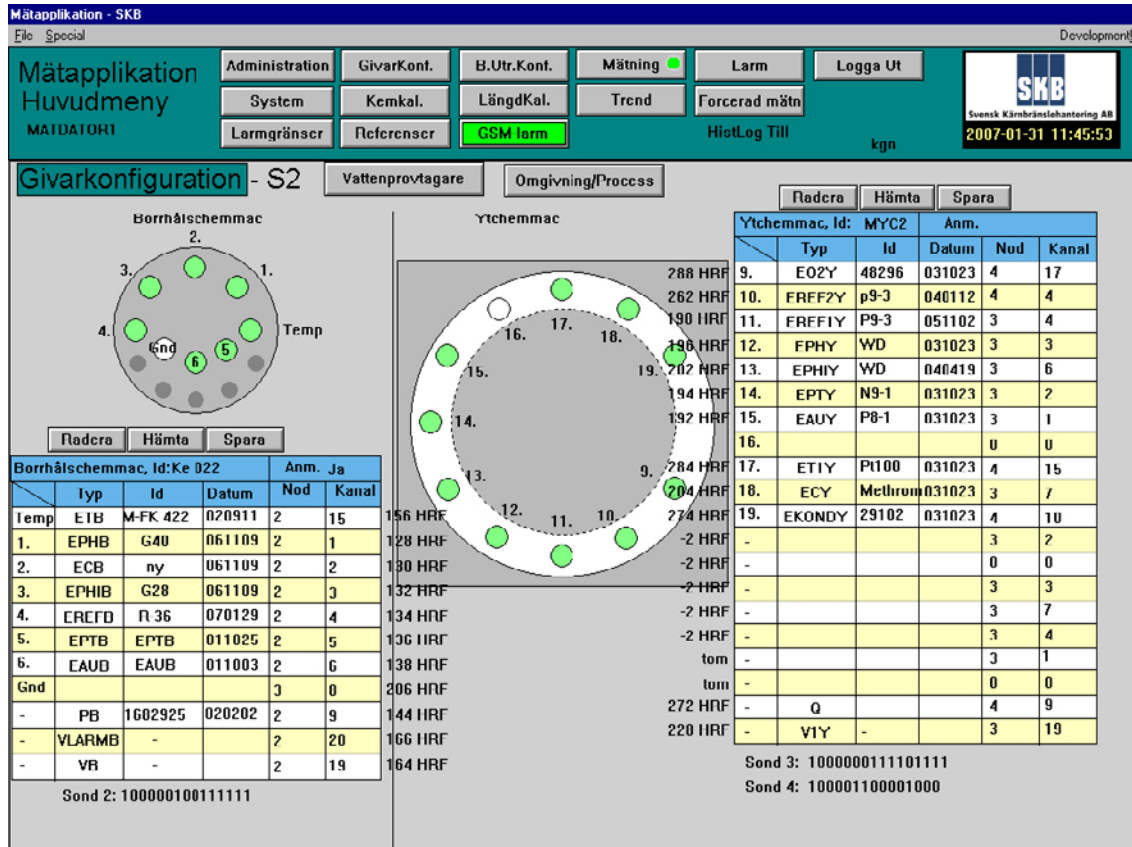


Figure A4-5. Electrode configuration, section 642.0–701.1 m.

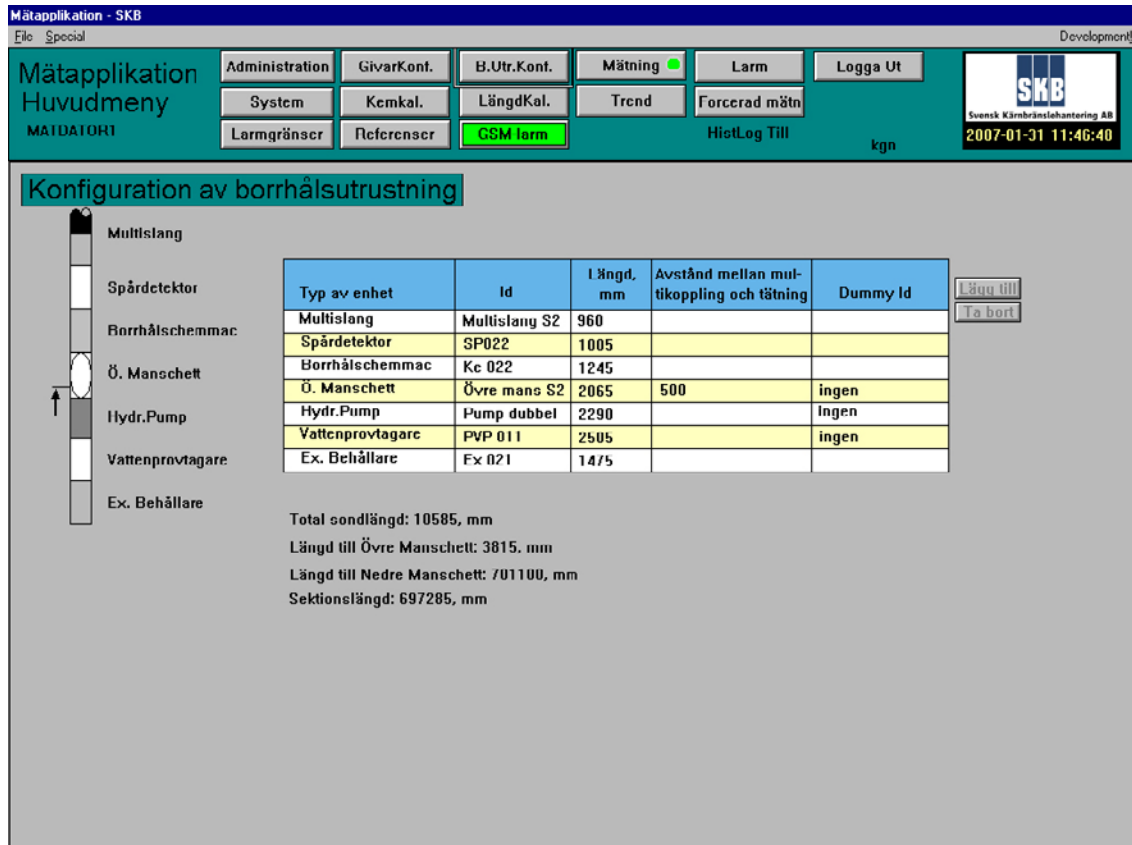


Figure A4-6. Configuration of downhole equipment, section 642.0–701.1 m.

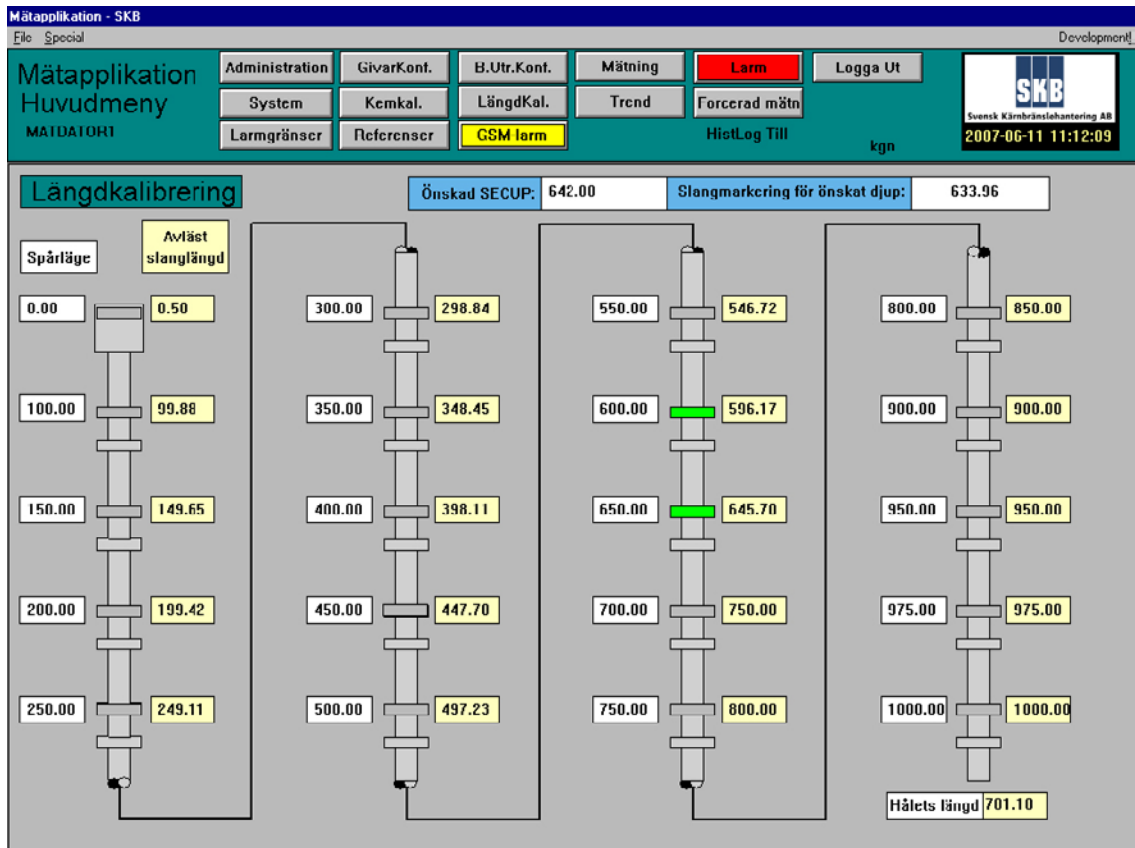


Figure A4-7. Length calibration, section 642.0–701.1 m.

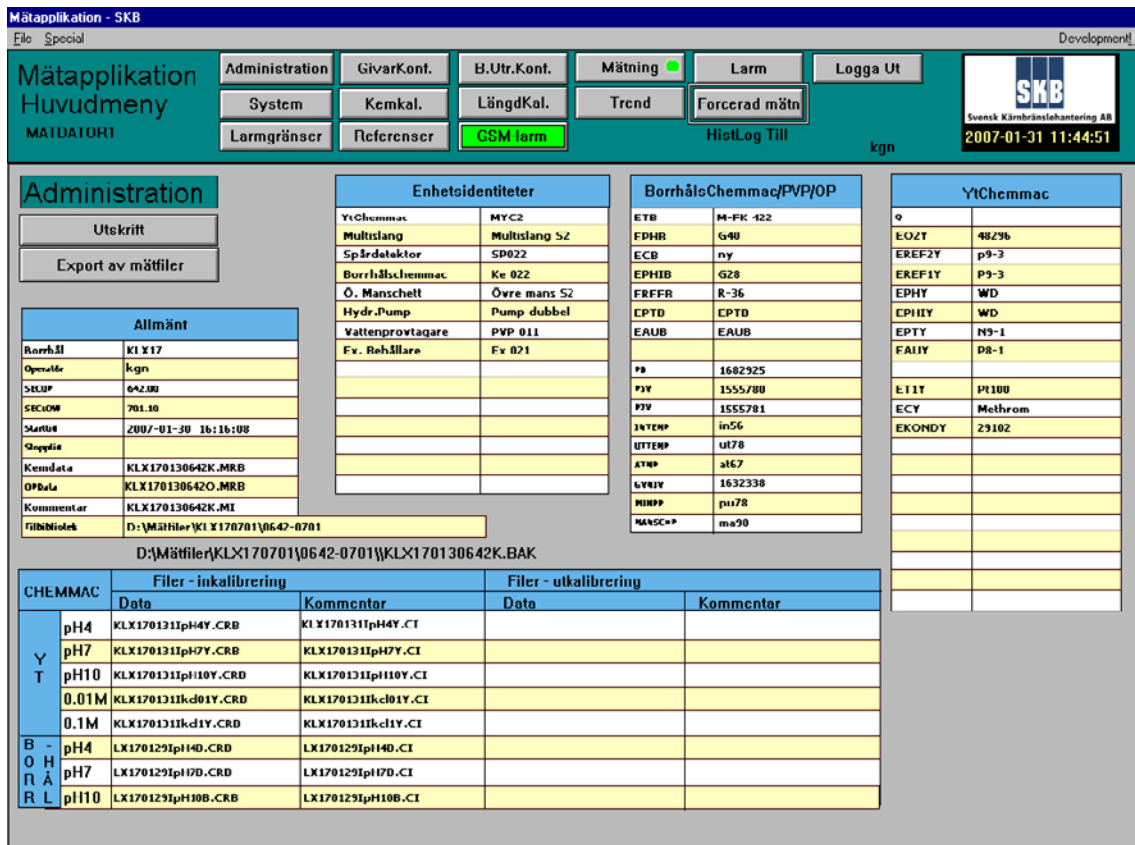


Figure A4-8. Administration, section 642.0–701.1 m.

Flow and pressure measurements in KLX17A

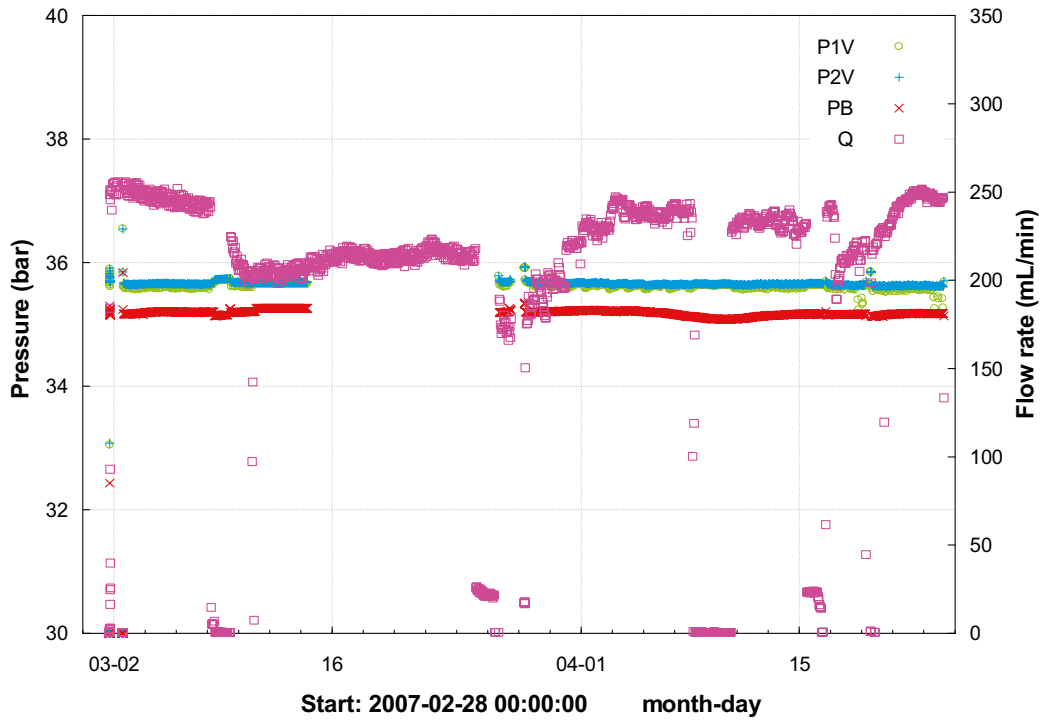


Figure A5-1. Pressure (P1V, P2V and PB) and flow rate (Q) measurements in borehole section 416.0–437.5 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. PB is the sensor in the borehole Chemmac and measures the pressure above the section.

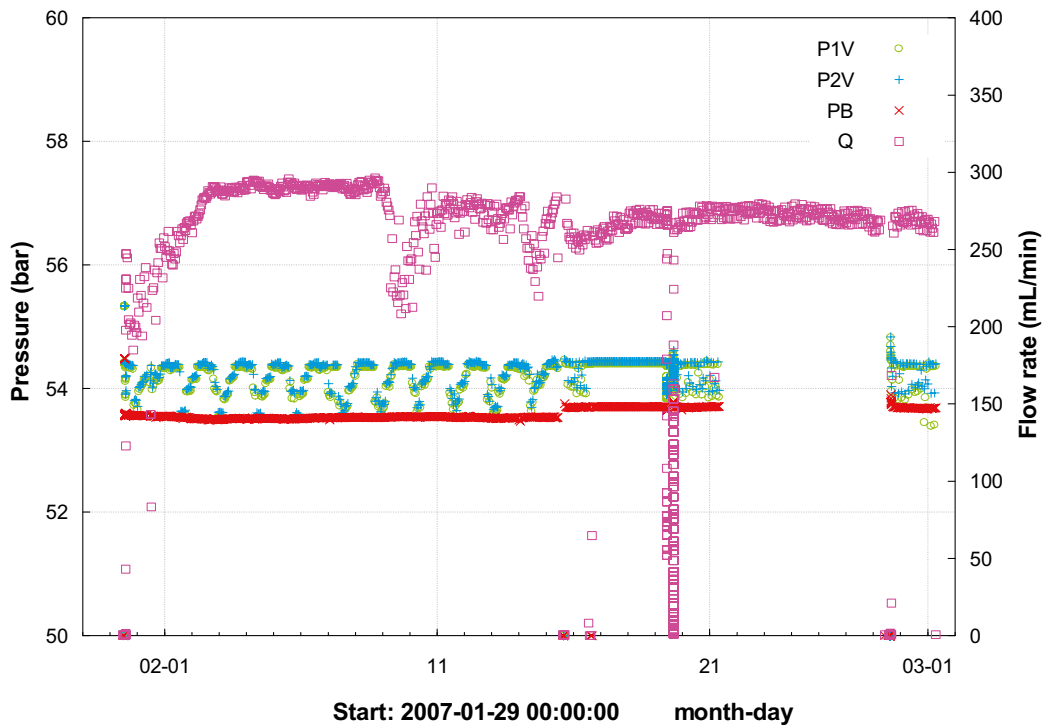


Figure A5-2. Pressure (P1V, P2V and PB) and flow rate (Q) measurements in borehole section 642.0–701.1 m. The P1V and P2V pressure sensors are placed in the in situ sampling unit and measure the pressure in the section. PB is the sensor in the borehole Chemmac and measures the pressure above the section.

Chemmac measurements in KLX17A, section 416.0–437.5 m

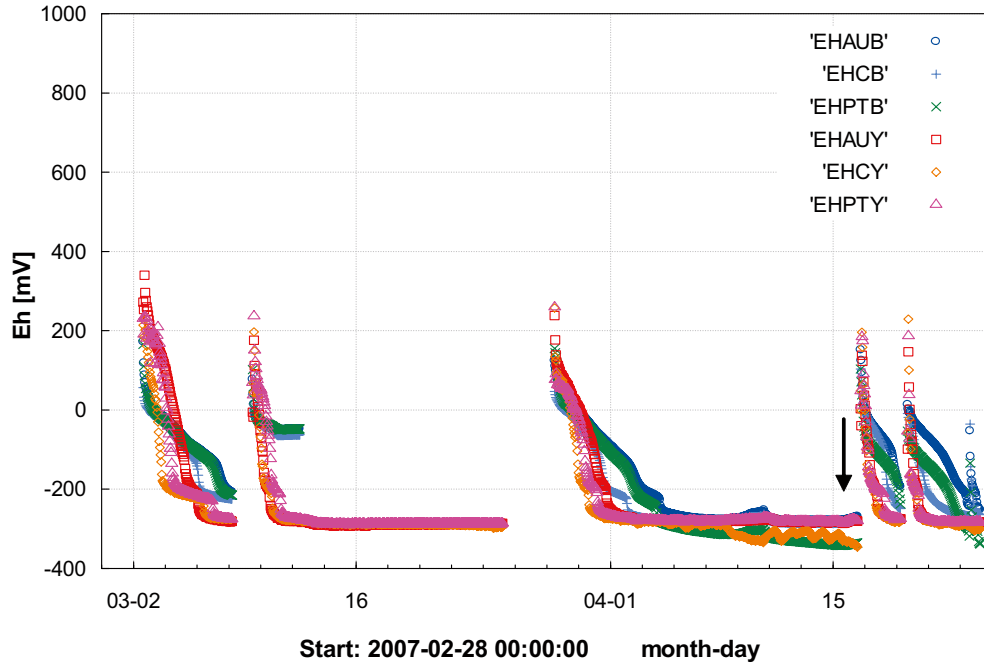


Figure A6-1. Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes in the borehole section (EHAUB, EHCB and EHPTB) and at the surface by gold, glassy carbon and platinum (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.

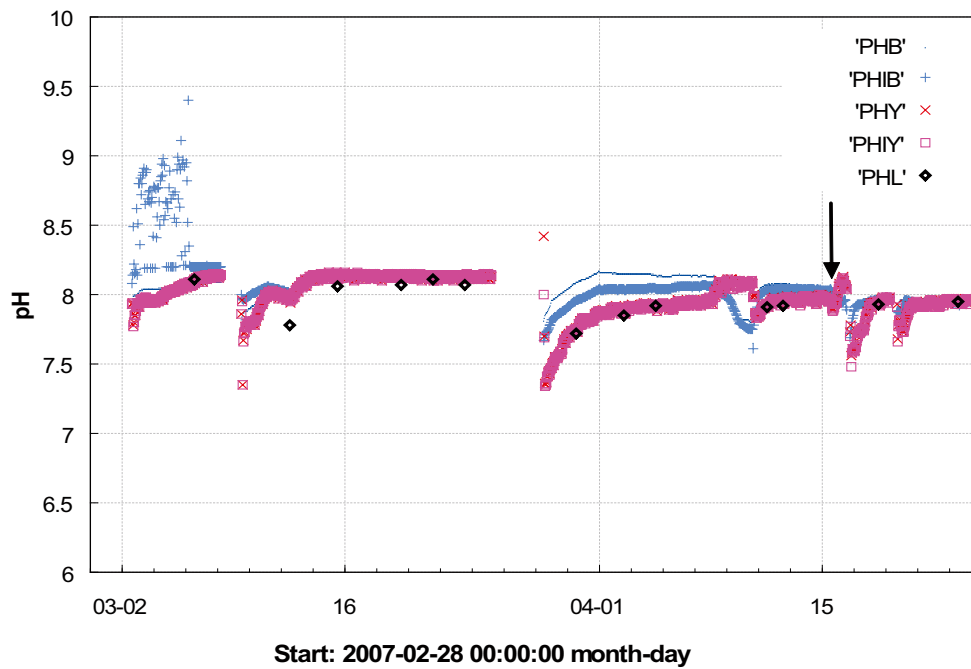


Figure A6-2. Measurements of pH by two glass electrodes in the borehole section (PHB and PHIB) and two glass electrodes at the surface (PHY and PHIY). The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.

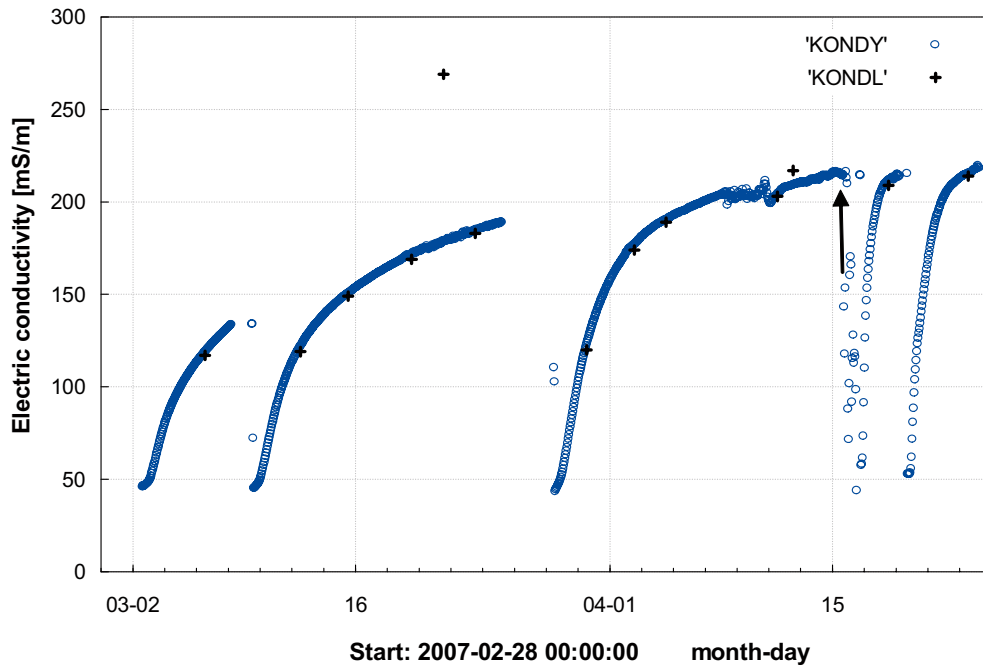


Figure A6-3. Electric conductivity measurements in the surface Chemmac cell (KONDY). The laboratory conductivity in each collected sample (KONDL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.

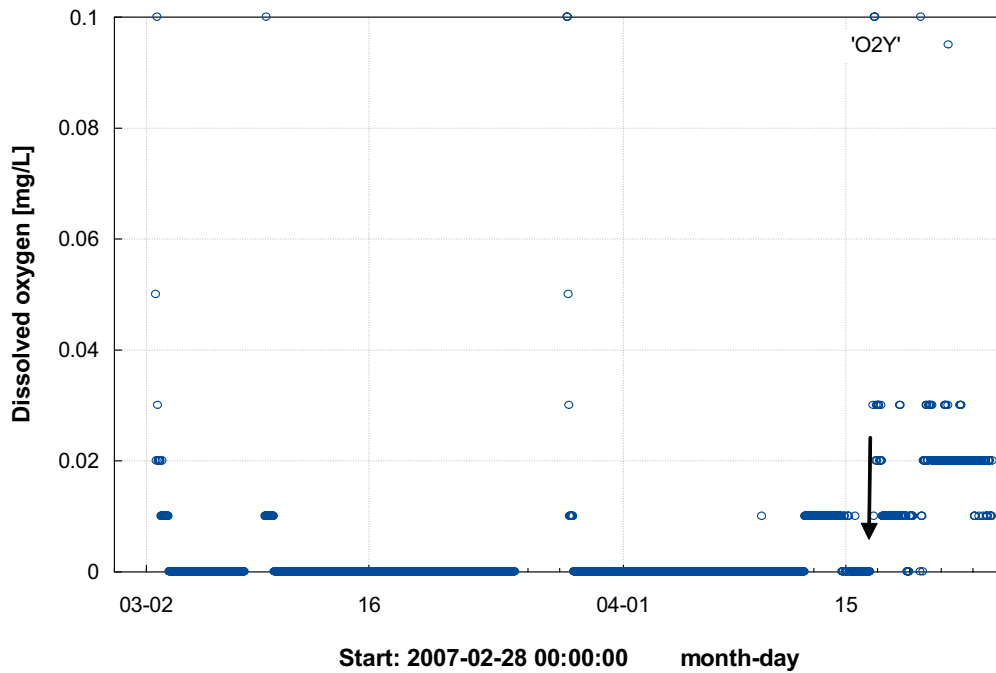


Figure A6-4. Dissolved oxygen measurements (O2Y) in the surface measurement cell. The arrow shows the chosen representative oxygen value for the borehole section.

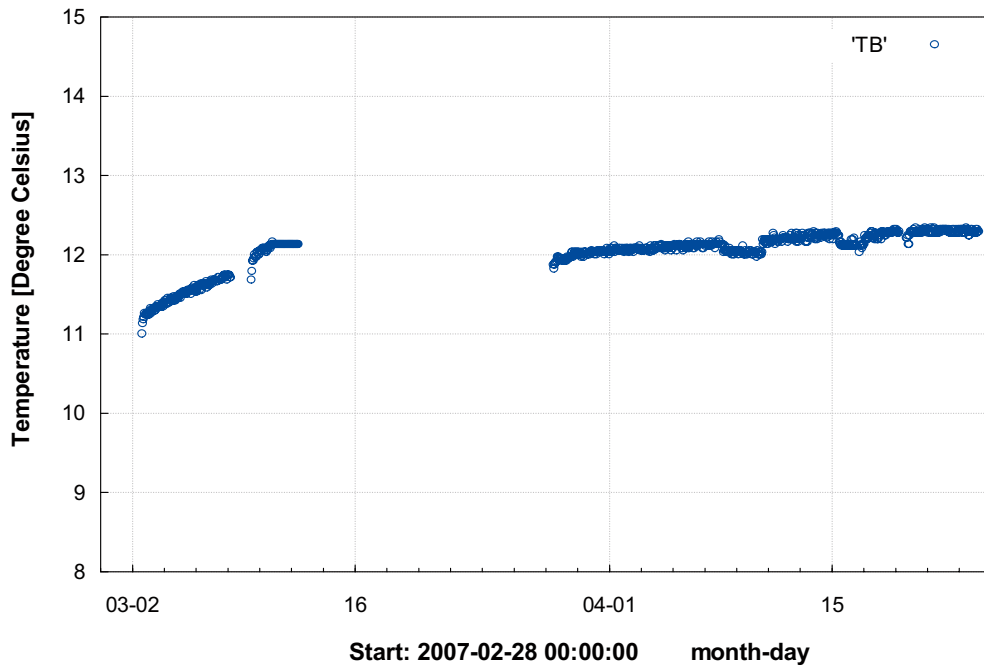


Figure A6-5. Temperature of the groundwater in the borehole section (TB).

Chemmac measurements in KLX17A, section 642.0–701.1 m

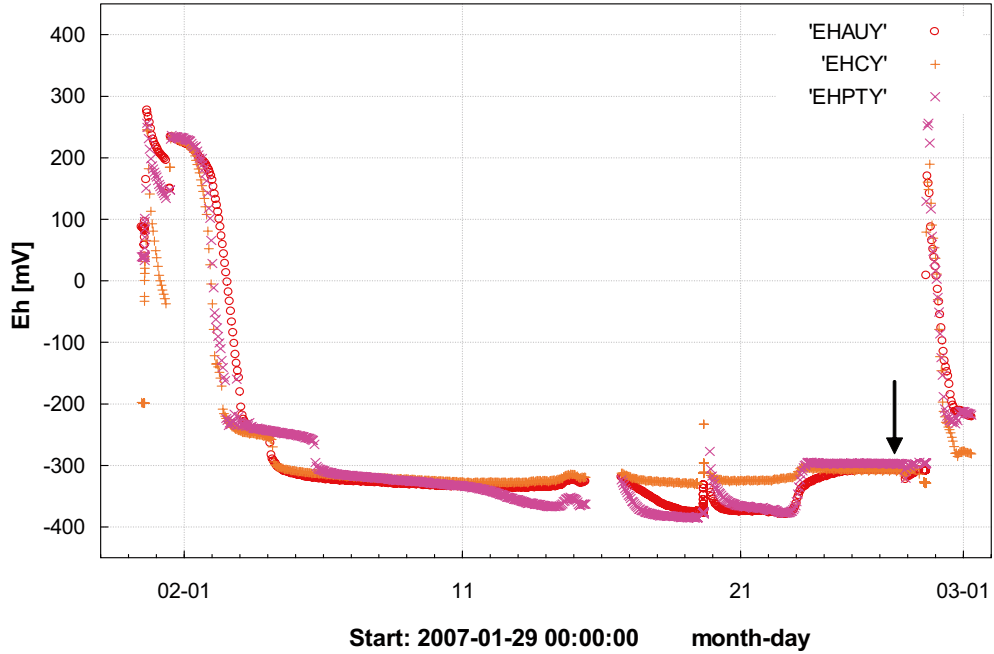


Figure A7-1. Redox potential measurements (Eh) by gold, glassy carbon and platinum electrodes at the surface (EHAUY, EHCY and EHPTY). The arrow shows the chosen representative Eh values for the borehole section.

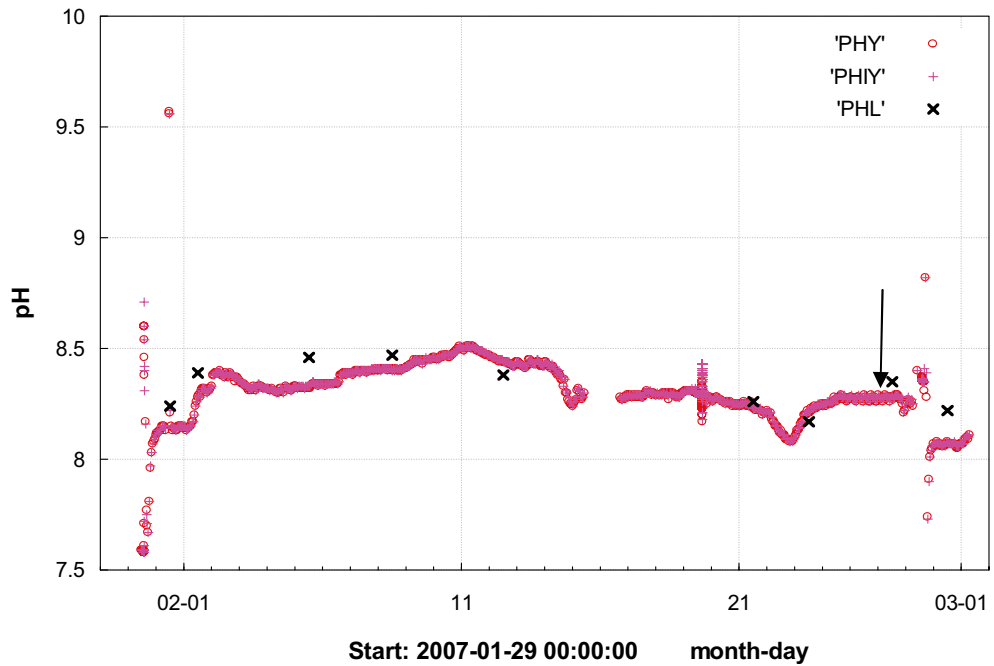


Figure A7-2. Measurements of pH by two glass electrodes at the surface (PHY and PHIY). The laboratory pH in each collected sample (PHL) is given for comparison. The arrow shows the chosen representative pH values for the borehole section.

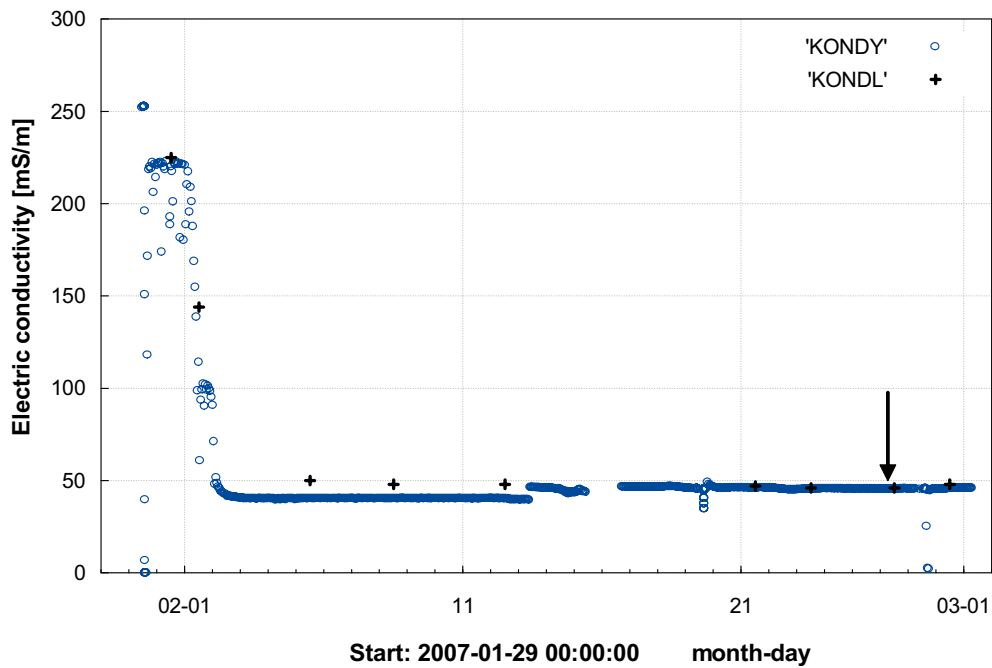


Figure A7-3. Electric conductivity measurements in the surface Chemmac cell (KONDY). The laboratory conductivity in each collected sample (KONDNL) is given for comparison. The arrow shows the chosen representative electric conductivity value for the borehole section.

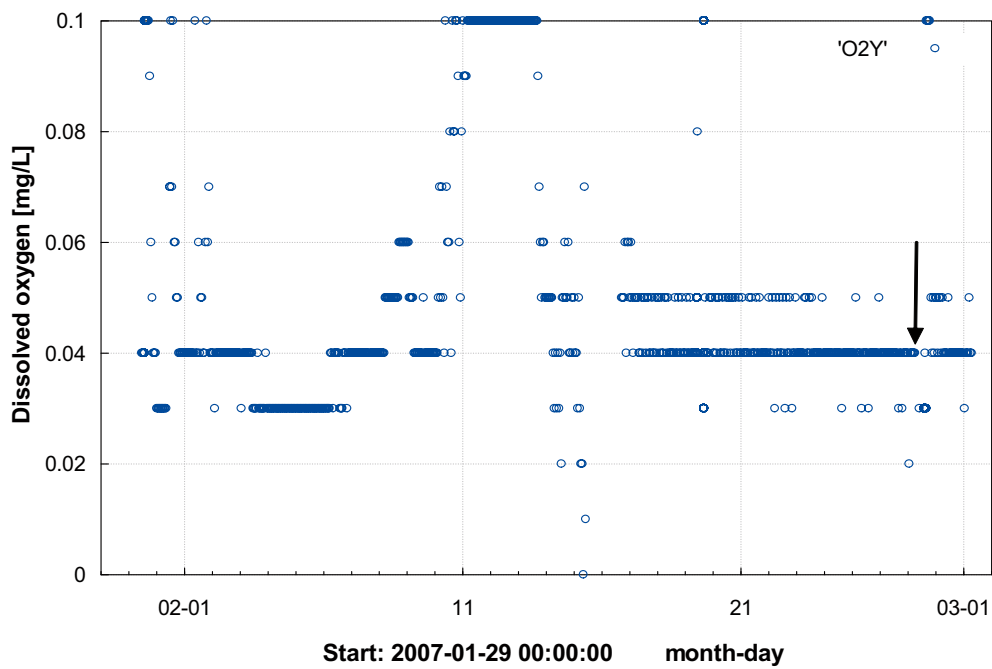


Figure A7-4. Dissolved oxygen measurements (O2Y) in the surface measurement cell. The arrow shows the chosen representative oxygen value for the borehole section.

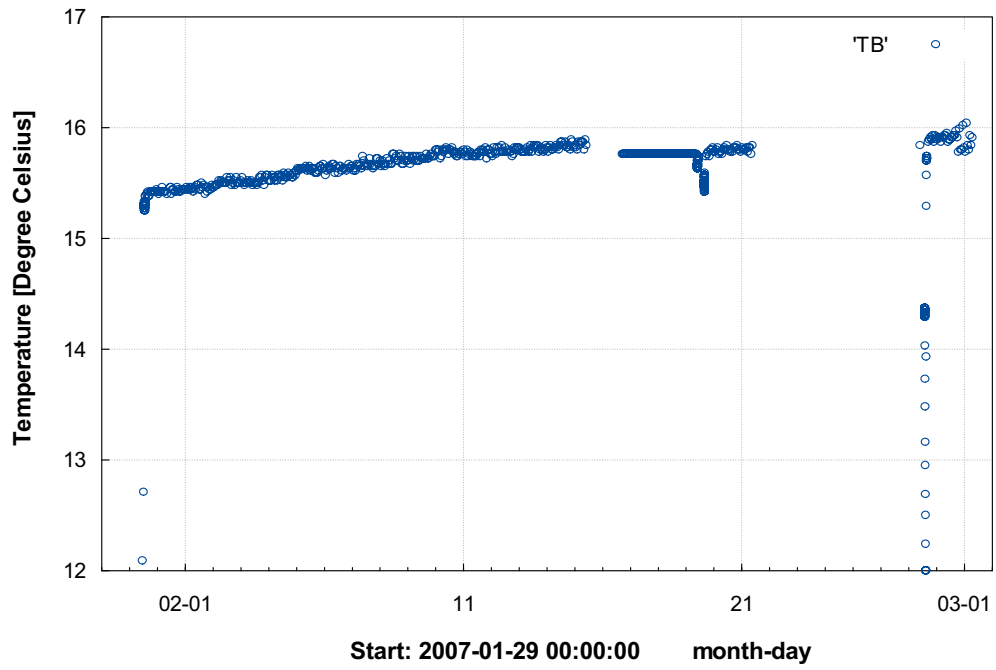


Figure A7-5. Temperature of the groundwater in the borehole section (TB).

Quantification of Colloids in Natural Groundwater from Laxemar Boreholes KLX13A, Section (432–439.2) m and KLX17A, Sections (642–701) m and (416–437.5) m

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P.O. Box 3640, D-76021 Karlsruhe, Germany

Introduction

Colloid analysis has been performed in groundwater samples collected during the site investigation program at Laxemar (Oskarshamns kommun), close to the nuclear power station Oskarshamn, Sweden. Samples from two boreholes and different sampling sections have been collected in stainless steel cylinders, preventing as much as possible the oxidation of the anoxic groundwater samples. They were sent to INE for laboratory analysis. Colloid analysis was subsequently performed by the laser-induced breakdown detection (LIBD) in the laboratory using a closed flow-through detection cell, again without atmosphere contact. Furthermore, a complete geochemical analysis of the water samples was performed.

It is supposed that the geological situation is similar to that found at various places in the Äspö tunnel. The aim of this study is to investigate the natural background colloid concentration in this specific boreholes and to compare the data with those obtained from other sites.

Experimental

LIBD instrumentation

The principle of LIBD is based on the generation of a dielectric breakdown in the focus region of a pulsed laser beam. As the threshold energy (irradiance) to induce a breakdown is lower for solids than for liquids or gas, the breakdown can be generated selectively in particles dispersed in solution at a suitable pulse energy.

A schematic diagram of the mobile LIBD set-up used in the present work is shown Figure A8-1. A pulsed laser beam with a frequency of 15 Hz at 532 nm wavelength from a small Nd:YAG-laser (Continuum Minilite I) is focused (15 mm focal length) into the center of a flow-through detection cell, after passing through a variable attenuator and a beam splitter. The plasma generated at a breakdown event is monitored by a microscope equipped with a CCD monochrome camera triggered by the incident laser pulse and recorded by a PC controlled image processing system. A breakdown shock wave propagated in the sample solution is detected simultaneously by an acoustic sensor (piezoelectric transducer) that is connected to the surface of the cell. Both, the energy and the acoustic signal are recorded by an analog-digital converter interface in a PC. Colloid concentrations are derived from the respective breakdown probability, represented by the number of breakdown events per number of laser shots, and the range of breakdown events within the laser beam axis determined by optical inspection of the laser focus area within the flow through cell. Colloid number concentrations (N/ml) are given relative to a calibration with polystyrene reference colloids. Mass concentrations are calculated by assuming an average colloid density of 2.7 g/cm³ and spherical particle shape. A more detailed description of data evaluation is given in 1.

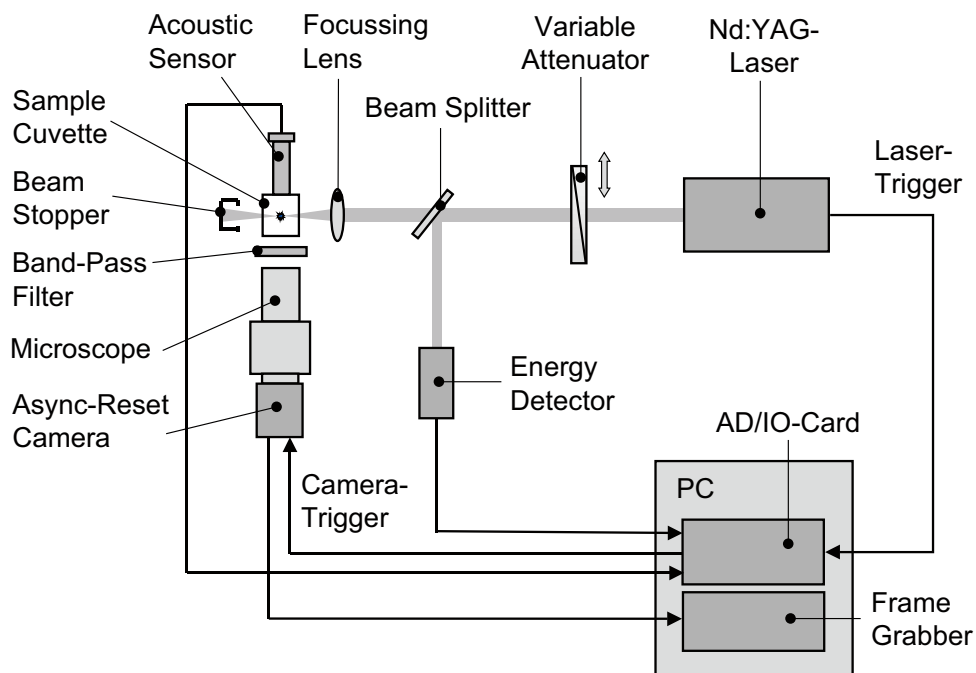


Figure A8-1. Schematic diagram of the mobile laser-induced breakdown detection system.

The mobile instrumentation of LIBD is combined with a Millipore ultra-pure water processing unit for on-line cleaning the flow-through detection cell of LIBD and to allow for the frequent control of the instrument background. The whole system, which is set up to a compact mobile unit can be transported by a van for field experiments.

High-pressure flow-through detection cell

The LIBD has been operated in the CRR migration experiments (Grimsel Test-Site, Switzerland) /1/ under low pressure conditions with commercially available quartz detection cells (fluorescence cells) for batch (laboratory experiments) or flow-through sampling. These cells have a sample volume of 3 ml at 10 mm absorption length. A new flow-through detection cell has been developed constraining water pressures of about 35 bar for in situ investigations in the Äspö Hard Rock Laboratory access tunnel (Sweden) 2, and in the Kraftwerke Oberhasli (KWO) access tunnel close to the Grimsel Test Site 3. This detection cell has also been applied in connection with a borehole sampling system for the detection of groundwater colloids sampled at a natural analogue site (Ruprechtov, Czech Republic).

Figure A8-2 presents the high-pressure detection cell developed by INE. Without changing the optical path of the laser light, the detection cell fits into the same mount used for the silica cell. The new cell, fabricated from PEEK (polyether etherketone) is lined outside with a stainless steel housing (black parts in Figure A8-2). Four optical windows, one at each side are applied for the passing laser light (absorption length 12 mm), the microscope and for inspection. They consist of sapphire with 2 mm thickness. The groundwater flow enters the inner cell volume of 0.8 ml from the base via a PEEK tubing. The outlet is on the top of the cell. The high-pressure detection cell is successfully tested for a water pressure up to 60 bar.

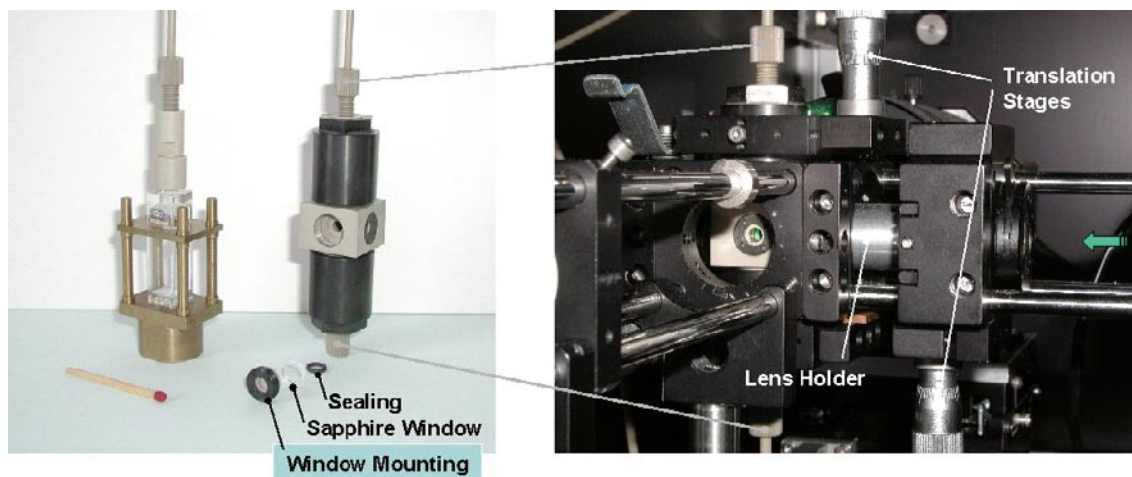


Figure A8-2. LIBD high-pressure flow-through detection cell (left: conventional flow-through silica detection cell).

Borehole sampling

Samples were taken

... at January 22, 2007 from Laxemar borehole KLX13A, section between (432–439.16) m. The vertical depth was approximately 430 m with a measured pressure in the borehole section of 42 bar. The samples are filled in the SKB steel cylinders PVB 203 and PVB 025.

... at February 27, 2007 from Laxemar borehole KLX17A, section between (642–701) m. The vertical depth was (548.6–600) m with a measured pressure in the borehole section of 54 bar. The samples are filled in the SKB steel cylinders PVB 201 and PVB 9506-1.

... at April 24, 2007 from Laxemar borehole KLX17A, section between (416–437.51) m. The vertical depth was (361–379) m with a measured pressure in the borehole section of 35 bar. The samples are filled in the SKB steel cylinders PVB 024 and PVB 9506-4.

The stainless steel cylinders (Figure A8-3) are groundwater sampling cylinders from SKB with a sample volume of about 190 ml each. They are supplied with an internal piston and 3 valves. Further information concerning the sampling procedure is given elsewhere (SKB).

In general one day after sampling the cooled samples arrived at the INE where they have been stored in a fridge (Temp. about 10°C) until colloid detection several days later.

Configuration of laboratory experiments

Each sampling cylinder was connected with the LIBD detection cell and the detection cells for pH-, Eh-, electrical conductivity-, oxygen content-detection and for taking samples for chemical groundwater analysis. As far as possible pressure resistant versions of the sensors are selected. In the specifications of the Eh- / pH- electrodes (Hamilton POLILYTE PLUS / POLILYTE PRO) a maximum groundwater pressure of 50 bar is designated. The maximum pressure for the oxygen-detector (Mettler Toledo InPro 6900) is specified with 6 bar and the electrical conductivity-detector (InPro 7000-VP) is 34 bar.



Figure A8-3. SKB stainless steel sampling cylinder (left: piston side, right: mounting adapter side).

A scheme of the corresponding laboratory setup is plotted in Figure A8-4 with an image of the experimental configuration in Figure A8-5.

At first the tubings around the sampling cylinder are intensively cleaned by evacuation and flushing with Argon. Then a HPLC-pump is used to fill all tubings on the water side of the sampling cylinder with ultra-pure water and to set the water pressure according the hydrostatic pressure of the samples. This was the expected water pressure in the sampling cylinder. The gas side of the sampling cylinder is then filled with the corresponding Argon gas pressure.

Now one of the top valves of the sampling cylinder can be opened without contact of the sampled groundwater with atmospheric oxygen. With Argon gas the groundwater is pressed out from the sampling cylinder through the LIBD detection cell via a degasser to avoid occasionally occurring gas bubbles which interfere the colloid detection. Behind the LIBD system additional detection cells with pressure resistant electrodes for Eh, pH (back pressure regulator 1 set to 40 bar), Oxygen, a sensor for electrical conductivity and a sensor for the pressure detection are arranged downstream.

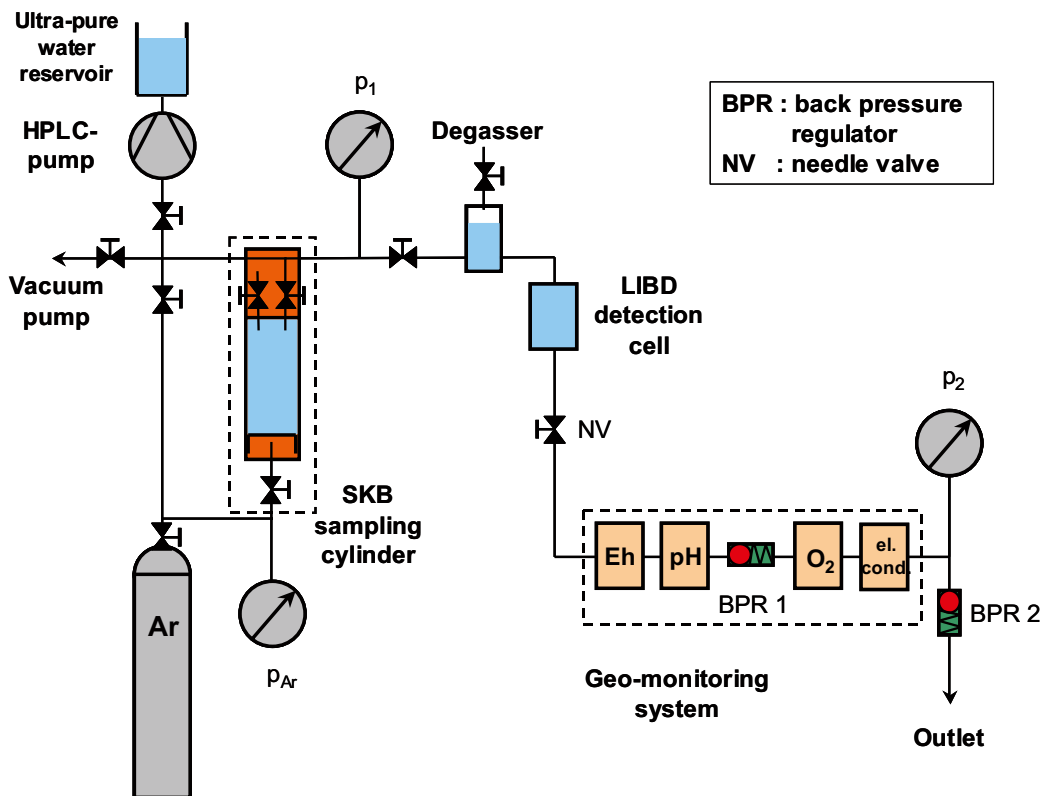


Figure A8-4. Scheme of the laboratory setup for in-line LIBD colloid analysis and groundwater monitoring.



Figure A8-5. Experimental configuration.

Before the sampling outlet an additional back pressure regulator, set to 5 bar, is installed. This overpressure in the whole system avoids further contact to oxygen. Data of this geo-monitoring system are stored on a personal computer with a data logger as a function of time. This allows to separate temporary fluctuating data, especially during the starting period when the detection cell and the geo-monitoring system are contaminated and do not contain the sampled groundwater, respectively.

Groundwater batch samples are collected at the outlet of the pressure regulator for chemical analysis with ICP-AES, ICP-MS and for the detection of inorganic carbon (IC) and dissolved organic carbon (DOC).

Additionally, track-etched Polycarbonate filter samples (pore size 50 nm) have been taken for colloid analysis with SEM/EDX.

Results

Chemical analysis

Data from geo-monitoring as well as the chemical composition of six samples (two from the same groundwater) are displayed in Table A8-1.

The groundwater pH of (8.0–8.5) is equivalent to the pH detected so far in other Forsmark (7.3–8.4) and Äspö groundwater samples (7.3–7.8). In the experiments only for groundwater KLX17A (416–437.5) m the Eh could be detected. Due to the malfunction of the electrode the other Eh-values have not been detected. They are calculated with PHREEQC assuming that $1 \cdot 10^{-7}$ mol/l of the Fe_{tot} measured is in the form of ferric iron. This assumption is based on the pH dependent solubility for iron oxides/hydroxides given in /4/.

Additionally, the oxygen values (Table A8-1) demonstrate that geochemical conditions are maintained within all sampling containers during transport, storage and colloid detection. This indicates that a significant intrusion of atmosphere oxygen did not occur. In two groundwater containers an oxygen concentration of ~0.010 mg/l was detected. As these detected values are slightly higher than the sensors detection limit (0.001 mg/l) it might be caused by sensor instabilities (see logged raw data) during the measurement.

All three Laxemar groundwaters are determined by their low Cl⁻-content of 20 mg/l and 750 mg/l, respectively. Whereas the chemical composition of Äspö and Forsmark groundwater is mainly characterized by the salinity from 3,000 to 14,000 mg/l chloride. The Laxemar DOC is comparable to the DOC of the Äspö groundwater KR0012B of the same salinity /5/.

It is supposed that differences in the K⁺-concentration of different samples of the same groundwater (Table A8-1: LX5A, LX6A), might be caused by a K⁺-contamination from the electrode storage solution, or a bleeding of Eh- / pH-sensor gel into the analyzed sample (... similar for differences in the SO₄²⁻-concentration (Table A8-1: LX3B, LX4C))

Table A8-1. Monitored data of pH, Eh, el. conductivity, oxygen content and chemical analysis of the groundwater samples from Laxemar boreholes KLX13A, KLX17A.

Borehole ID		KLX13A		KLX17A		KLX17A	
Secup - Seclow	m	432 - 439.16		642 - 701		416 - 437.5	
Sampling depth	m	~ 420		548.6 - 600.1		361 - 379	
Hydr. pressure	bar	42		54		35	
Container ID		SKB PVB 203	SKB PVB 025	SKB PVB 201	SKB PVB 9506-1	SKB PVB 024	SKB PVB 9506-4
Sample ID		LX1A	LX2A	LX3B	LX4C	LX5A	LX6A
pH		8.2	8.5	8.45	8.39	8.1	7.94
Redox (Ag/AgCl)	mV	[-209]	[-260]	[-286]	[-278]	-237	-217
Eh (SHE)	mV	[5]	[-46]	[-72]	[-64]	-23	-3
el. cond.	mS/m	256	256	51	58	224	220
O ₂ content	mg/l	<0.011	<0.008	<0.002	<0.001	<0.029	<0.015
Na ⁺	mg/l	438	423	93.1	89.3	327	314
K ⁺	mg/l	11.3	9.46	8.4	7.51	23.4	7.96
Ca ²⁺	mg/l	49.1	48.2	12.2	12.2	72.9	72.4
Mg ²⁺	mg/l	2.68	2.71	2.31	2.21	9.7	9.7
Al ²⁺	mg/l	0.01	0.01	0.05	0.04	6.95	6.95
HCO ₃ ⁻ (a)	mg/l	69.5	70.5	231	229	106.2	106.3
Cl ⁻	mg/l	750	762	17.4	21.9	758.1	679.2
SO ₄ ²⁻	mg/l	27.8	22.6	3.78	1.51	21.1	20.7
Br ⁻	mg/l	3.98	3.6	<0.1	<0.1	2.7	2.3
F ⁻	mg/l	7.1	5.4	2.75	3.89	2	2.1
Si ⁴⁺	mg/l	4.74	4.89	<0.001	<0.001	6.9	7.06
Fe-ICP	mg/l	0.086	0.078	0.37	0.4	0.216	0.233
Mn ²⁺	mg/l	0.02	0.02	0.03	0.04	0.08	0.08
Li ⁺	mg/l	0.07	0.07	0.016	0.016	0.05	0.05
Sr ²⁺	mg/l	4.74	4.89	6.73	6.88	2.3	2.35
DOC	mg/l	16.5	13.9	16.85	21.44	24.8	20.9
IC	mg/l	13.7	13.9	45.5	45	8.3	21

(a) calculated from IC

[] Redox, Eh calculated with PHREEQC

Colloid analysis

Groundwater from KLX13A (432–439.16) m

Data determined with the laser-induced breakdown detection system are listed in Table A8-2. The volume of the samples was sufficient to perform four or five colloid measurements for each PVB container (see logged raw data). So temporal variations in the colloid concentration during the elution of the groundwater can be detected.

After evaluation of image processed data colloid size distributions with two main average colloid fractions are derived. A 1st colloid fraction with diameters of 60–110 nm with corresponding mass concentrations of 2–5 µg/l are calculated. During the elution of container PVB 203 a higher colloid concentration of 40 µg/l is detected. This might be caused by mobilized larger colloids (diameter 356 nm) which previously have settled down on the container bottom (piston surface).

1,100–1,400 nm particles with mass concentrations of 680–1,380 µg/l are the main part of the 2nd colloid fraction. This 2nd fraction contains more than 99% of the total particle mass, whereas the total colloid number density is determined of the 1st (smaller) colloid fraction.

Table A8-2. LIBD data with average colloid diameter and colloid concentration of the analyzed groundwater from Laxemar borehole KLX13A, (432–439.16) m.

Borehole ID		KLX13A					KLX13A			
Secup - Seclow	m	432-439.16					432-439.16			
Sampling depth	m	~ 420					~ 420			
Hydr. pressure	bar	42					42			
Container ID		SKB PVB 203					SKB PVB 025			
LIBD /det. ID		LX1A	LX1B	LX1C	LX1D	LX1E	LX2A	LX2B	LX2C	LX2D
Trigger-pulses		2000	2000	2000	2000	2500	2000	2000	2000	2000
1st coll. fraction (1):										
BD-events		366	324	365	204	260	286	186	151	
BD-probability		0.183	0.162	0.183	0.102	0.104	0.143	0.093	0.076	
coll. num. density	N/ml	3.2E+06	5.6E+06	6.3E+05	2.1E+06	1.5E+06	3.5E+06	2.0E+06	1.3E+06	
coll. diam.	nm	101	58	356	85	113	76	83	95	
coll. mass conc.	µg/l	5	2	40	2	3	2	2	2	
2nd coll. fraction (2):										
BD-events		964	892	783	759	976	807	936	943	1351
BD-probability		0.482	0.446	0.392	0.38	0.39	0.404	0.468	0.472	0.676
coll. num. density	N/ml	3.5E+05	3.9E+05	2.5E+05	2.8E+05	3.6E+05	3.9E+05	5.9E+05	7.5E+05	2.0E+06
coll. diam.	nm	1408	1200	1470	1302	1097	1076	910	757	559
coll. mass conc.	µg/l	1379	941	1121	875	677	683	626	462	485
Sum (1)+(2):										
coll. num. density	N/ml	3.5E+06	6.0E+06	8.8E+05	2.4E+06	1.9E+06	3.9E+06	2.6E+06	2.1E+06	2.0E+06
coll. mass conc.	µg/l	1384	943	1161	877	680	685	628	464	485

Figure A8-6 shows the corresponding SEM images of groundwater KLX13A (432–439.16) m colloids. It is evident that two major colloid fractions exist. A 1st small colloid fraction has a size ≤ 100 nm. This seems to be the component with the highest number density. The 2nd particle fraction (500–1,000) nm is the component with the lowest number density. Some particles seem to be agglomerates of the 1st fraction (Figure A8-6a, b).

In this case EDX element analysis was not possible because of the small quantities of colloidal material.

Groundwater from KLX17A (642–701) m

After starting the elution of groundwater KLX17A (642–701) m the LIBD detected breakdown probability increased from 0% to 100%. Even after 120 min. detection the breakdown probability did not decrease. The same effects occurred with the groundwater from both sampling cylinders PVB 201 and PVB 9506-1 (see logged raw data).

This means that the amount of particles is higher than LIBD can detect, or in other words LIBD is too sensitive for the given samples.

SEM images of this groundwater (Figure A8-7) show a big amount of colloids with diameter from about 100 nm, 300 nm, and more. Even bacteria are found. With EDX analyzed elements are Al, Si (alumino-silicates, silicates), F, Fe.

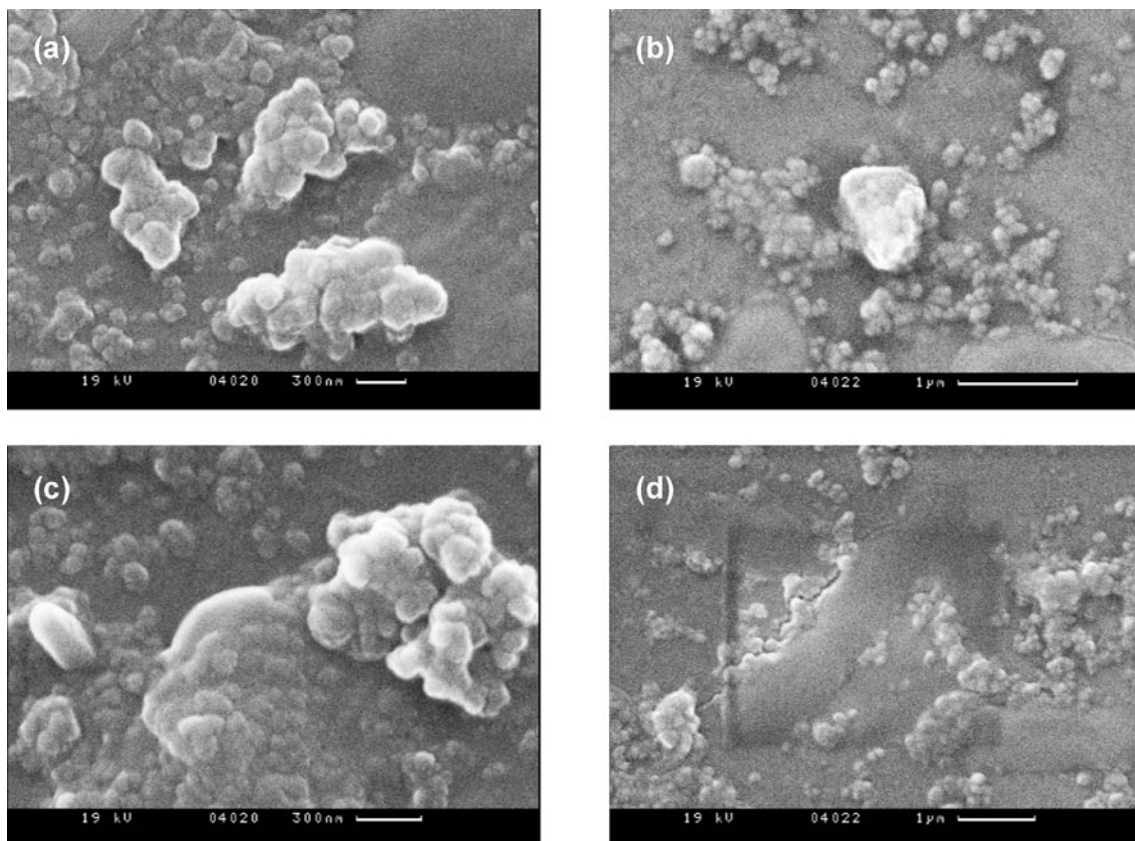


Figure A8-6. SEM images of groundwater KLX13A (432–439.16) m colloids on a 50 nm track-etched Polycarbonate filter.

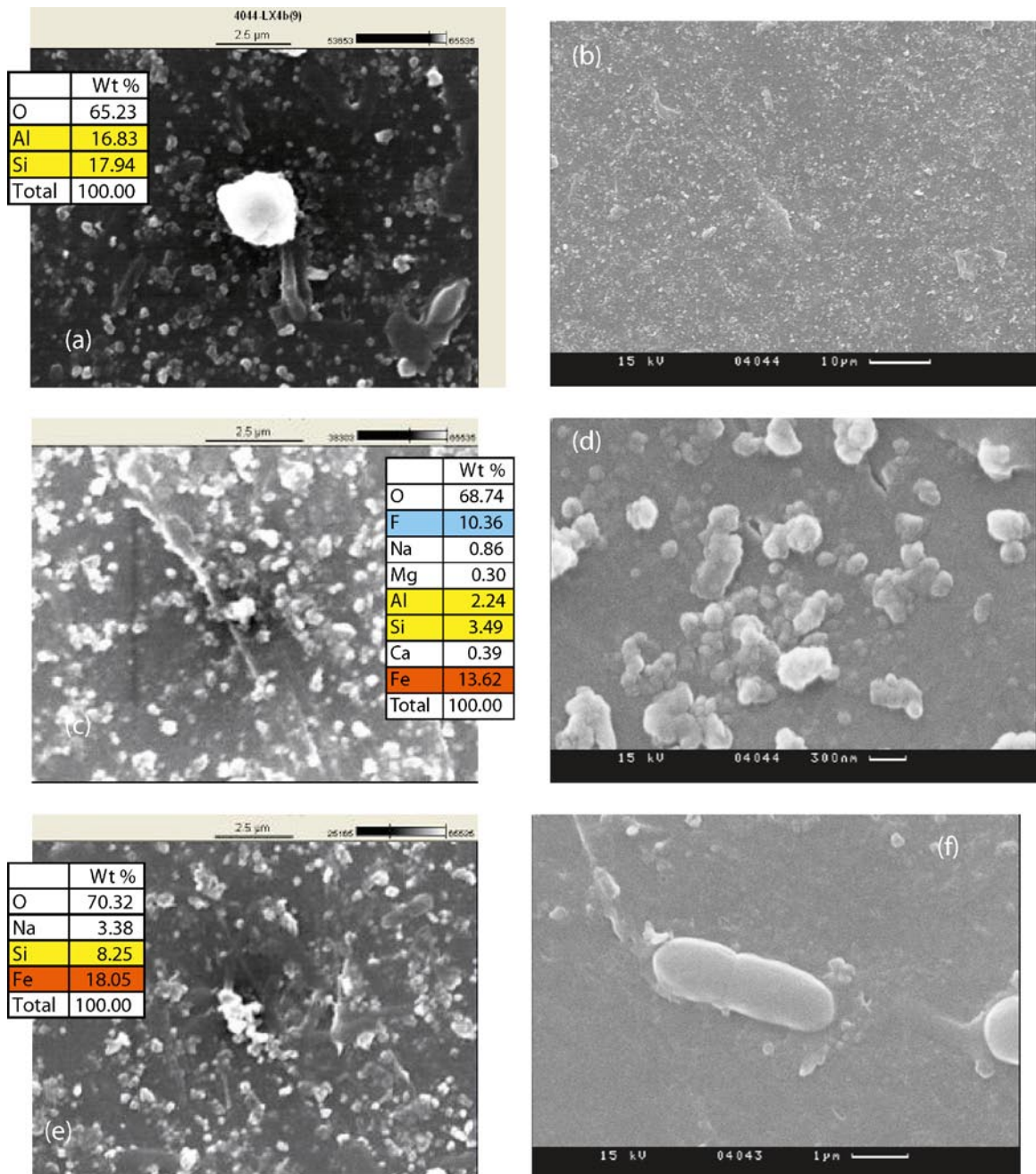


Figure A8-7. SEM images of groundwater KLX17A (642–701) m colloids on a 50 nm track-etched Polycarbonate filter.

Groundwater from KLX17A (416–437.5) m

The same borehole has been sampled again with two steel cylinders, but from about 200 m higher borehole sections. With each groundwater sample seven LIBD colloid measurements (Table A8-3) are performed, again to quantify temporal fluctuations caused by changing flow conditions.

During groundwater elution from SKB steel cylinder PVB 024 colloids with an average diameter between (360–470) nm and corresponding mass concentrations of (210–280) μg/l are detected. About a factor of 2 lower are the colloid mass concentrations of the same groundwater taken from steel cylinder PVB 9506-4.

Table A8-3. LIBD data with average colloid diameter and colloid concentration of the analyzed groundwater from Laxemar borehole KLX17A, (416–437.5) m.

Borehole ID		KLX17A				KLX17A			
Secup - Seclow	m	416-437.5				416-437.5			
Sampling depth	m	361-379				361-379			
Hydr. pressure	bar	35				35			
Container ID		SKB PVB 024				SKB PVB 9506-4			
LIBD /det. ID		LX5A	LX5B	LX5C	LX5D	LX6A	LX6B	LX6C	LX6E
BD-events		1266	1319	1286	1218	1053	1057	975	1373
Trigger-pulses		2000	2000	2000	2000	2000	2000	2000	3000
BD-probability		0.633	0.66	0.643	0.609	0.527	0.529	0.4875	0.458
coll. num. density	N/ml	2.7E+06	3.0E+06	3.2E+06	2.5E+06	3.0E+06	3.0E+06	2.1E+06	2.3E+06
coll. diam.	nm	398	388	359	402	289	291	350	306
coll. mass conc.	µg/l	241	248	208	230	104	106	129	94
LIBD /det. ID		LX5E	LX5F	LX5G		LX6F	LX6G	LX6H	
BD-events		1083	1174	1167		869	1089	1063	
Trigger-pulses		1769	2000	2000		1662	2000	2000	
BD-probability		0.612	0.587	0.584		0.523	0.545	0.532	
coll. num. density	N/ml	2.7E+06	1.9E+06	2.2E+06		3.6E+06	3.4E+06	2.5E+06	
coll. diam.	nm	382	470	425		254	279	341	
coll. mass conc.	µg/l	213	283	236		83	103	140	

This difference is significant and it is not clear where it comes from. Possible reasons can be

- differences in the degree of cleaning and flushing with inert gas of each steel cylinder before its use for sampling,
- differences of the filling procedure of the cylinders during sampling in the Laxemar borehole (e.g. erosion of additional colloids),
- ...

Corresponding SEM images in Figure A8-8 show colloids starting from a size around 100 nm (Figure A8-8 (f)). They look like agglomerates (Figure A8-8 (d)) of a basic form of colloids which was also found in other groundwater samples (Figure A8-6, Figure A8-7). Larger particles (several µm) consist of Si, Fe, Ca, Al / Si.

Comparison with Äspö and Forsmark data

In the Äspö colloid project /5/ a series of boreholes along the access tunnel have been sampled and their groundwater was directly analyzed with the mobile LIBD system. A correlation was drawn (Figure A8-9) between the colloid concentration and the Cl⁻ concentration of the groundwater. At a Cl⁻ concentration of about 4,000 mg/l a remarkable decrease of the colloid concentration over 4 orders of magnitude down to the LIBD detection limit of about 10 ng/l was observed.

The Forsmark KFM sample data from 307 m to 390 m sampling depth fits quite well into this correlation. According to the colloid concentration correlation with groundwater salinity we should expect lower colloid concentrations for samples KFM01D, KFM08A, and KFM08D from the deeper sampling depths 442 m, 590 m, and 663 m (Figure A8-9). Possible reasons for the somewhat high particle concentrations have been discussed in previous Forsmark reports.

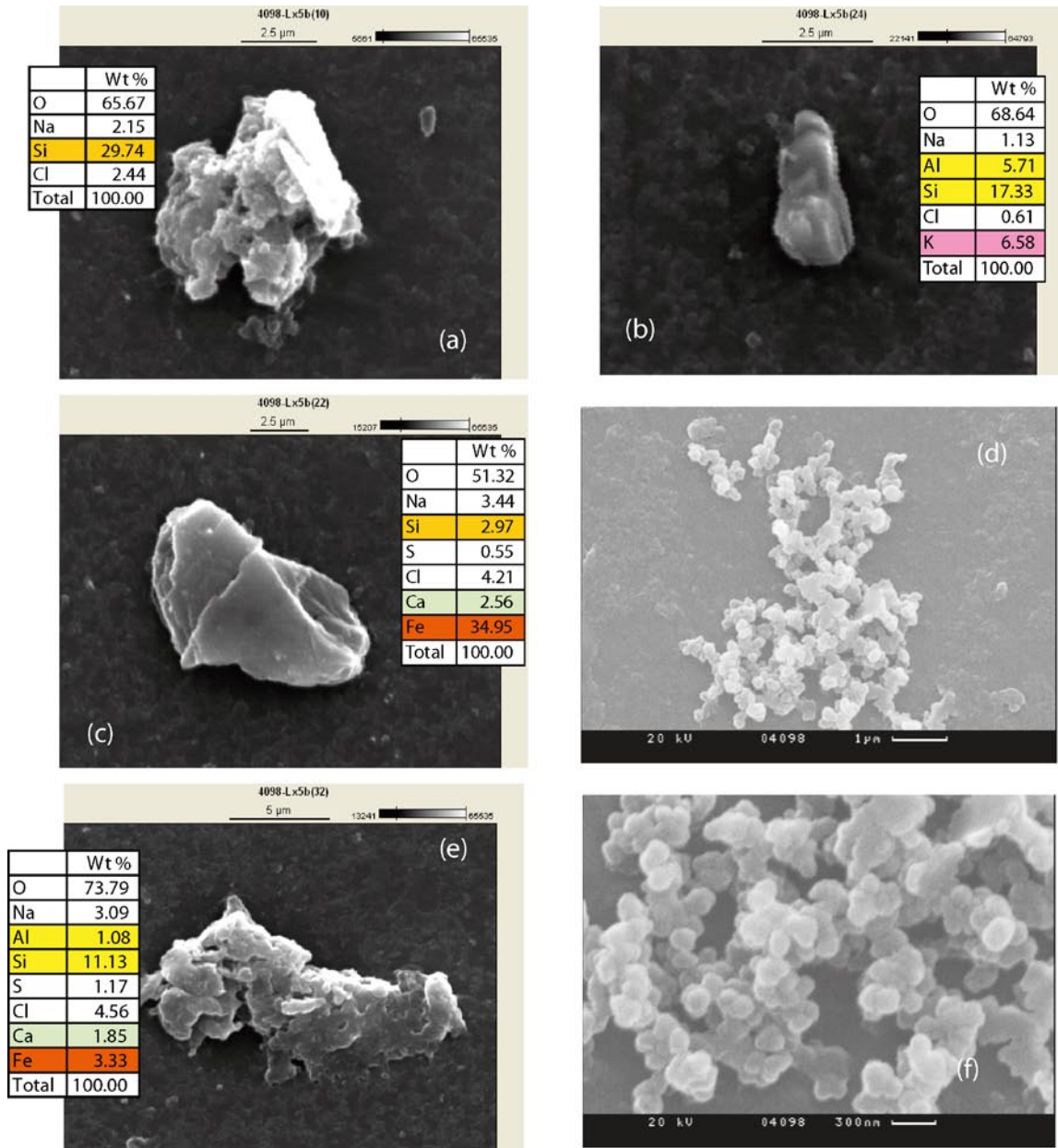


Figure A8-8. SEM images of groundwater KLX17A (416–437.5) m colloids on a 50 nm track-etched Polycarbonate filter.

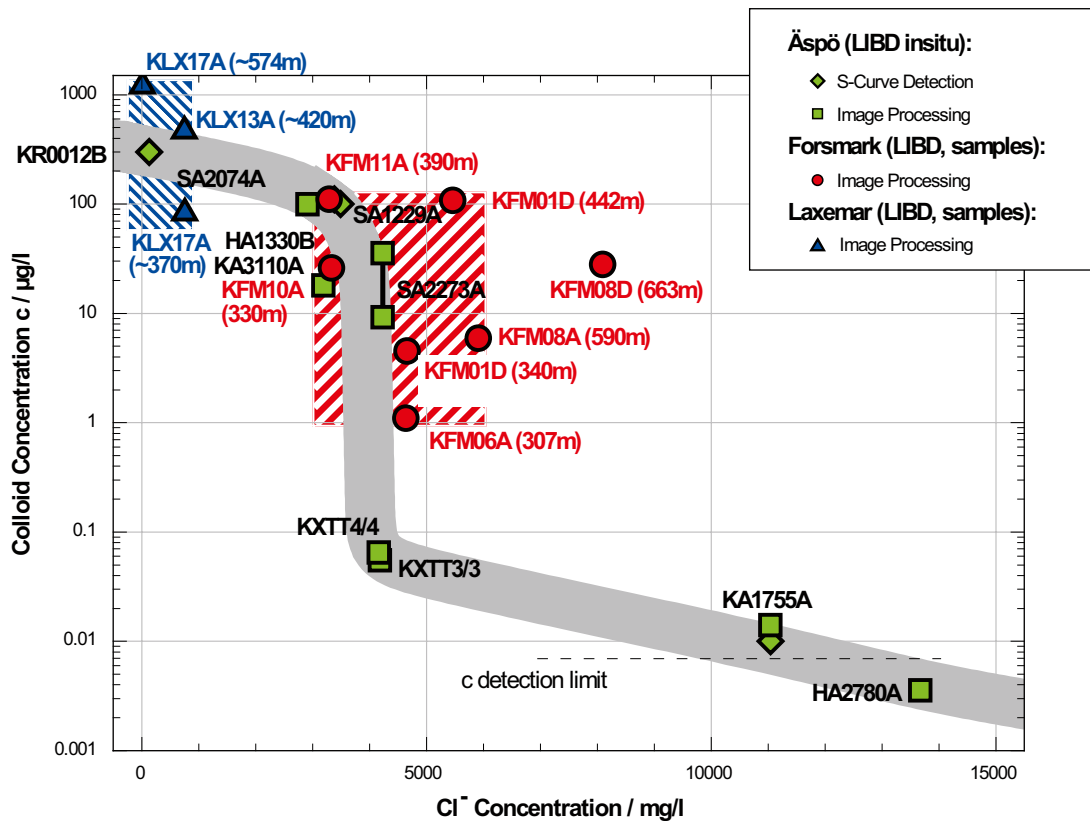
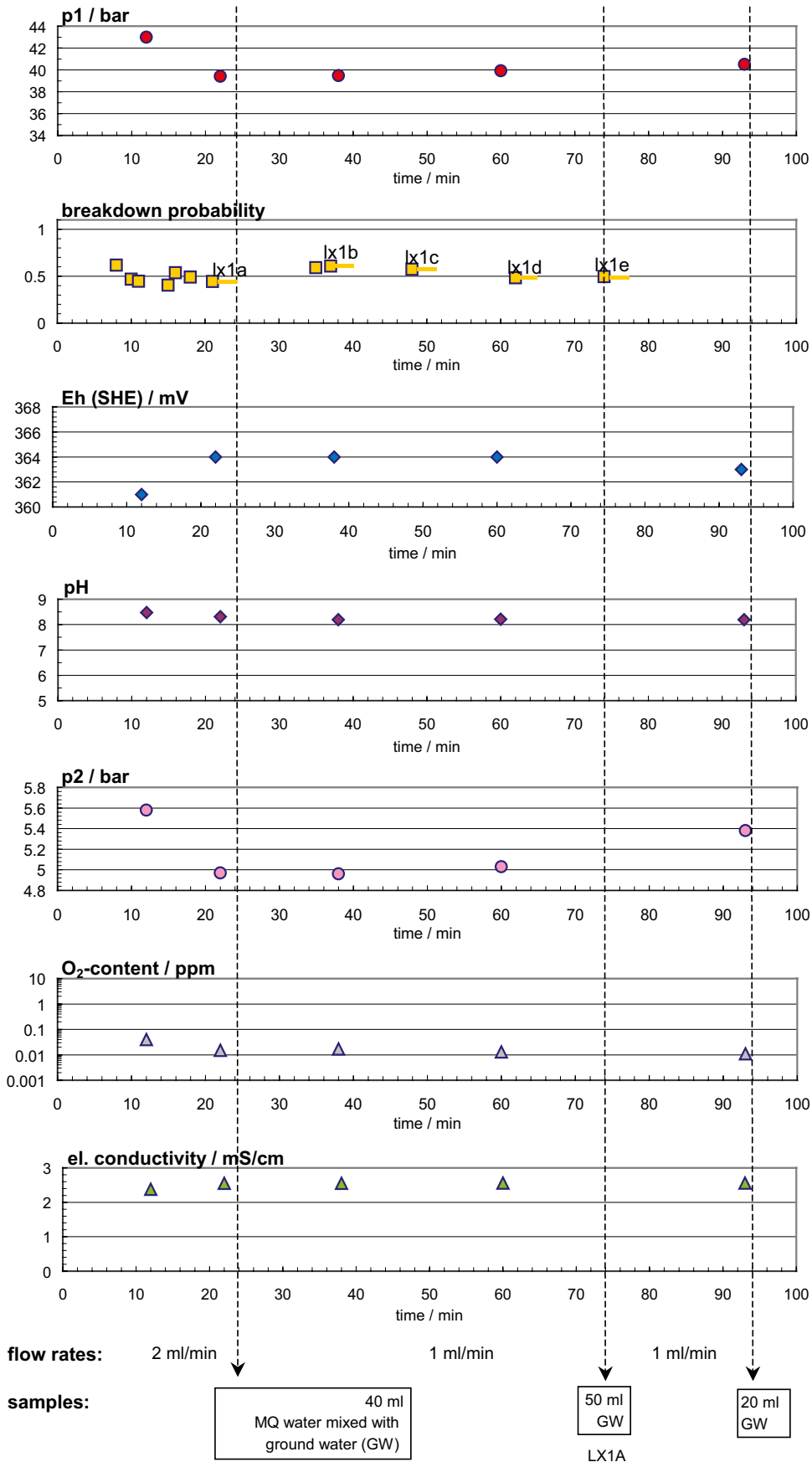


Figure A8-9. Correlation between colloid concentration and chloride concentration in different groundwater from Äspö 2, 5 and in Forsmark samples. (): sampling depths.

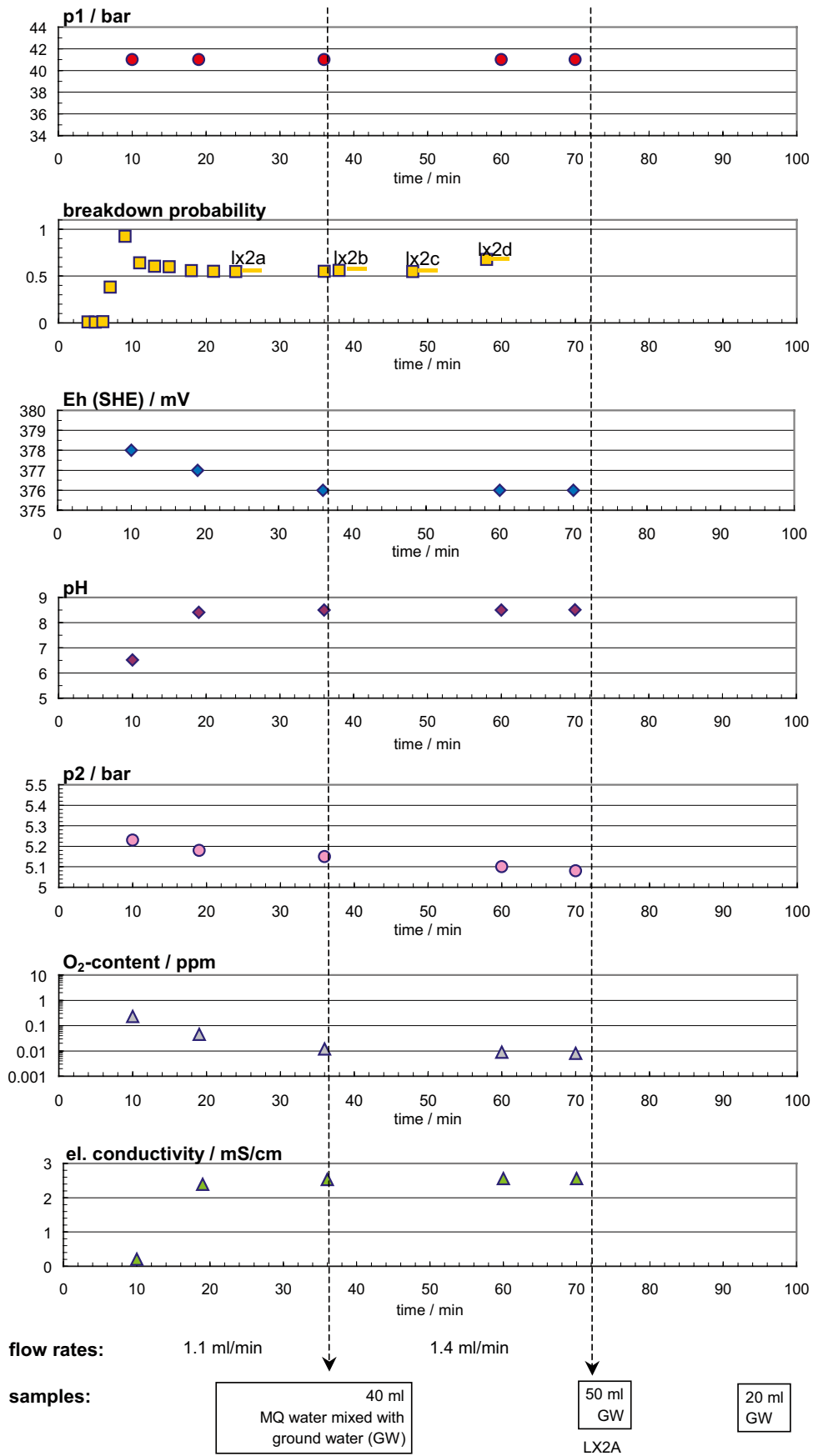
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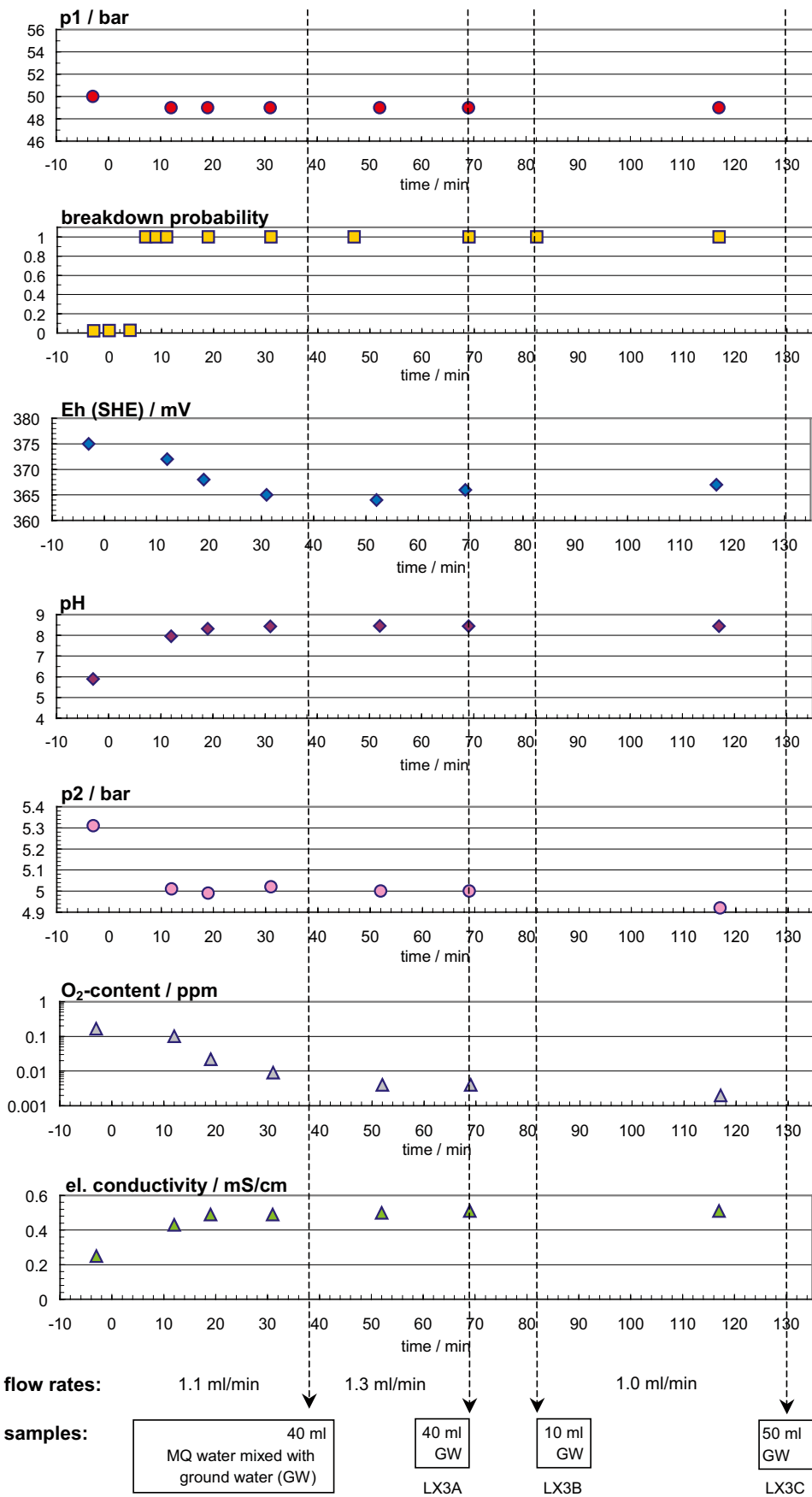
Logged raw data from elution of sampling container SKB PVB 203 (KLX13A (432-439.16m))



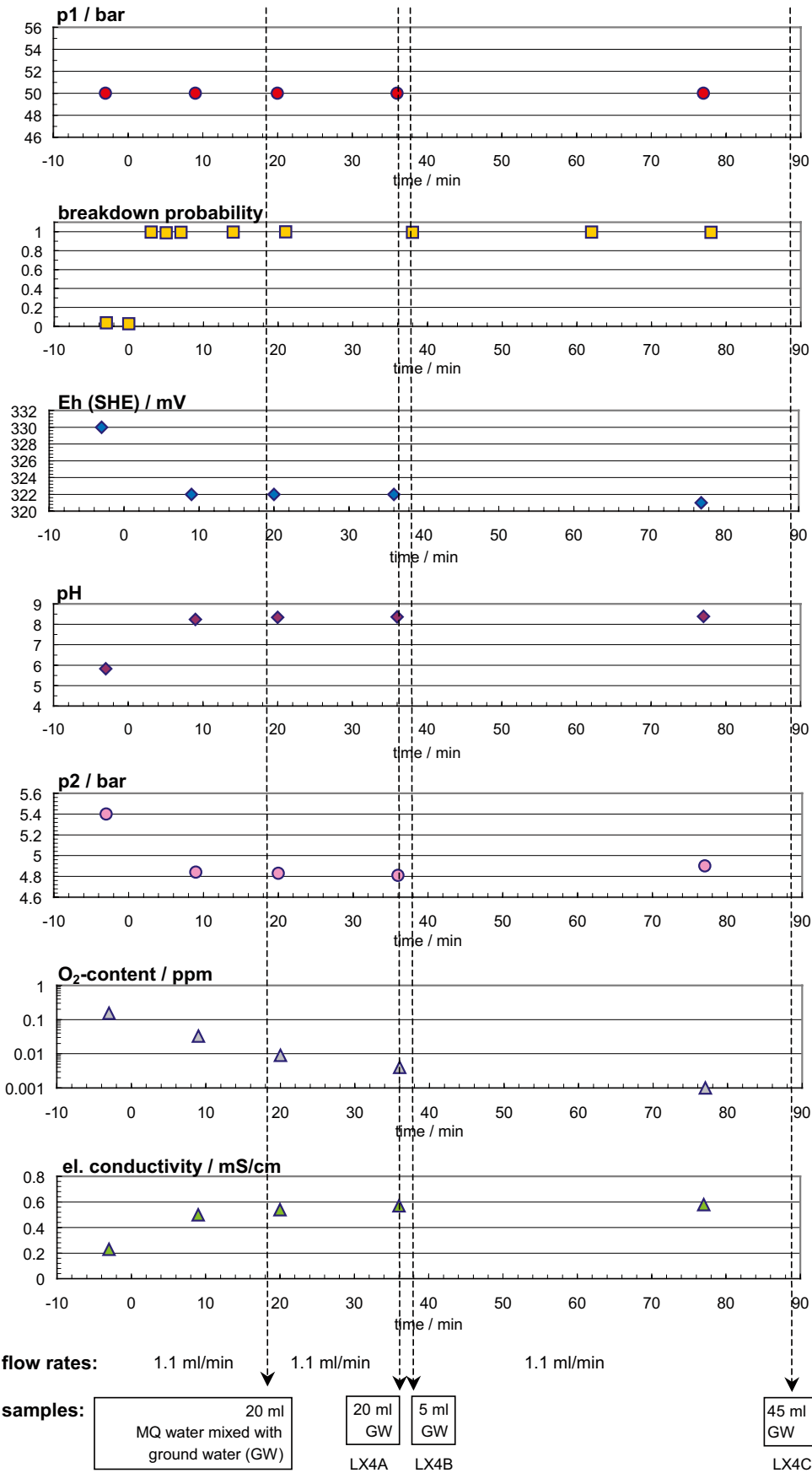
Logged raw data from elution of sampling container SKB PVB 025 (KLX13A (432-439.16m))



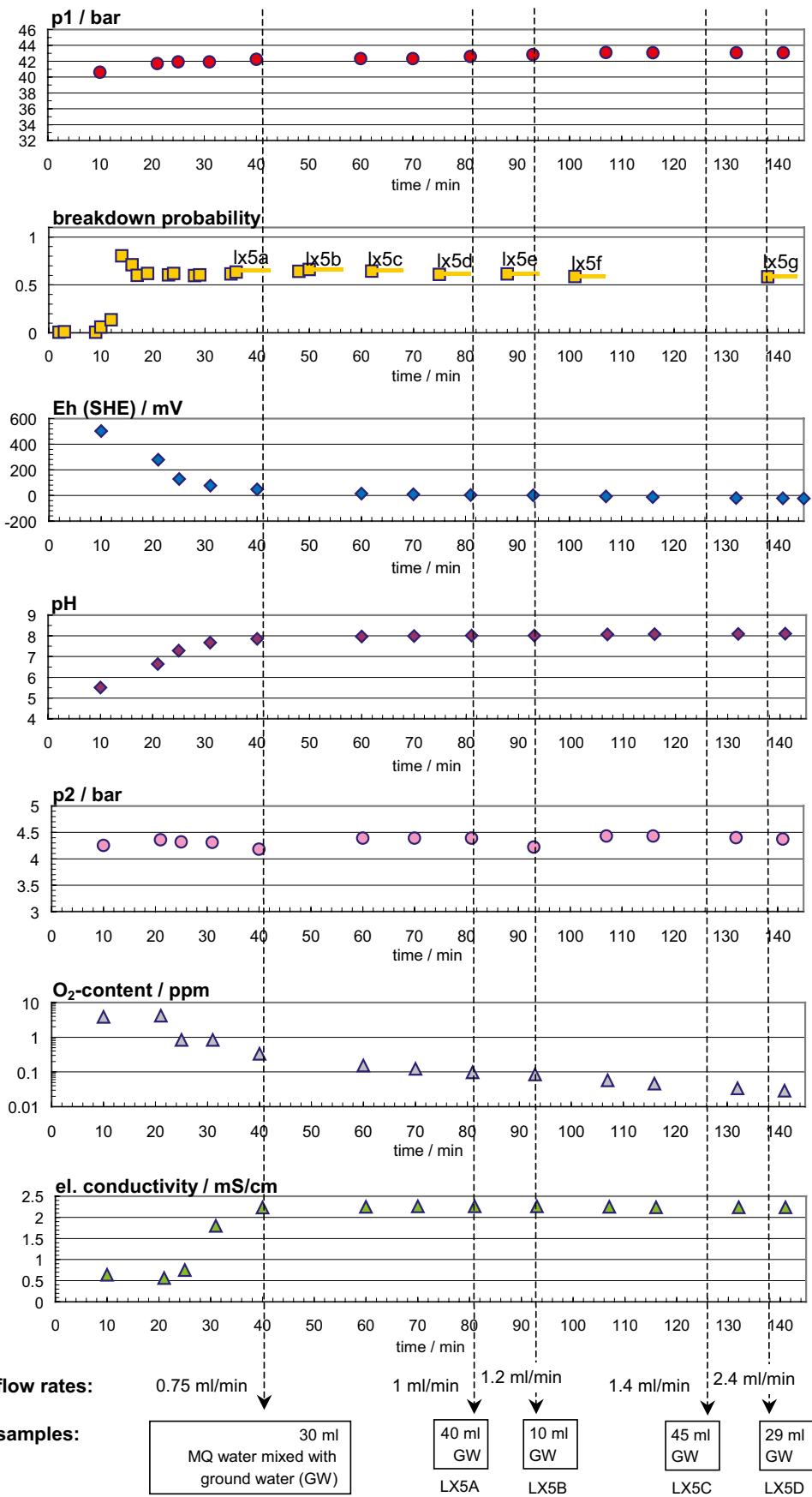
Logged raw data from elution of sampling container SKB PVB 201 (KLX17A (642-701m))



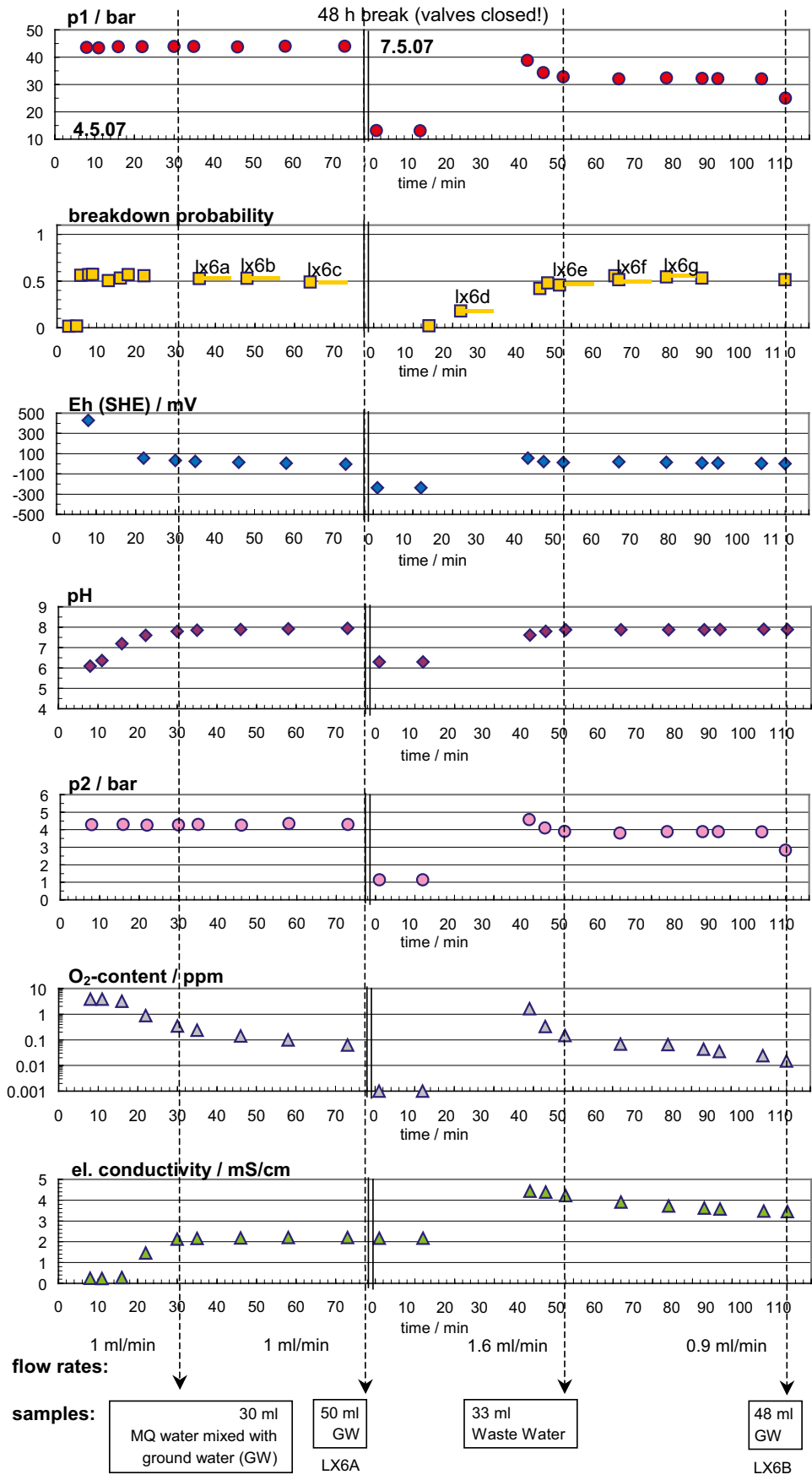
Logged raw data from elution of sampling container SKB PVB 9506-1 (KLX17A (642-701m))



Logged raw data from elution of sampling container SKB PVB 024 (KLX17A (416-437.51m))



Logged raw data from elution of sampling container SKB PVB 9506-4 (KLX17A (416-437.51m))



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	Analysis within – or delivery time to lab.
Drill water	Uranine	Glass (brown)	100	No	No	Spectro-fluorometry	–
Anions	HCO ₃ ⁻ pH (lab) cond. (lab)	Plastic	250	No	No	Titration Pot. meas. Cond. meas.	The same day – maximum 24 hours
	Cl ⁻ , SO ₄ ²⁻ , Br ⁻ , F ⁻	Plastic	250	Yes (in connection to the analysis)	No	Titration (Cl ⁻) IC (Cl ⁻ , SO ₄ ²⁻ , Br ⁻ , F ⁻) ISE (F ⁻)	Not critical (month)
	Br ⁻ (control sample to external laboratory)	Plastic	100	Yes	No	ICP MS	Not critical (month)
	I ⁻	Plastic	100	Yes	No	ICP MS	Not critical (month)
Cations etc	Na, K, Ca, Mg, S(tot), Si(tot), Fe, Mn, Li, Sr	Plastic (acid washed)	100	Yes	Yes (1 mL HNO ₃)	ICP AES ICP MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic-PEH (acid washed)	500	Yes	Yes (5 mL HCl)	Spectrophotometry Ferrozine method	As soon as possible the same day
Hydrogen sulphide	HS ⁻	Glass (Winkler)	About 120×2	Yes	1 mL 1 M NaOH+ 1 mL 1M ZnAc	Spectrophotometry	Immediately or if conserved, a few days
Nutrient salts	NO ₂ -N, NO ₃ -N+NO ₂ -N, PO ₄ -P	Plastic	250	Yes	No	Spectrophotometry	Maximum 24 hours
	NH ₄ -N	Plastic cylinder	50	No	No	Spectrophotometry	Maximum 24 hours
Environmental metals etc	Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn, In	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP AES ICP MS	Not critical (month)
Lanthanoids, U, Th, etc	Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP AES ICP MS	Not critical (month)
Dissolved organic Carbon	DOC	Plastic	250	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analyzer Shimadzu TOC5000	Short transportation time
Total organic Carbon	TOC	Plastic	250	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analyzer Shimadzu TOC5000	Short transportation time

Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/Conservation*	Analysis method	Analysis within – or delivery time to lab.
Environmental isotopes	$\delta^2\text{H}$, $\delta^{18}\text{O}$	Plastic	100	No	–	MS	Not critical (month)
Tritium,	^3H (enhanced.)	Plastic (dry bottle)	500	No	–	LSC	Not critical (month)
Chlorine-37	$\delta^{37}\text{Cl}$	Plastic	500	No	–	ICP MS	Not critical (month)
Carbon isotopes	$\delta^{13}\text{C}$, pmC (^{14}C)	Glass (brown)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	$\delta^{34}\text{S}$	Plastic	1,000	No	–	Combustion, ICP MS	No limit
Strontium-isotopes	$^{87}\text{Sr}/^{86}\text{Sr}$	Plastic	100	No	–	TIMS	Days or Week
Uranium and Thorium isotopes	^{234}U , ^{235}U , ^{238}U , ^{232}Th , ^{230}Th ,	Plastic	1,000	No	–	Chemical separat. Alfa/gamma spectrometry	No limit
Boron isotopes	$^{10}\text{B}/^{11}\text{B}$	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP MS	No limit
Radon and Radium isotopes	^{222}Rn , ^{226}Ra	Plastic	1,000	No	No	EDA, RD-200	Immediate transport
Dissolved gas (content and composition)	Ar, He, N_2 , CO_2 , O_2 , CH_4 , H_2 , CO , C_2H_6 , C_2H_4 , C_2H_2 , C_3H_8 , C_3H_6	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series and fractionation (Analysis of cations and environmental metals)	Polycarbonate filters	2.0, 0.4, 0.2 and 0.05 μm	–	Ar atmosphere	ICP AES ICP MS	Immediate transport
Density	Density	Plastic	250	No	–	Pycnometer	–
Archive samples with acid	–	Plastic (washed in acid)	100×2**	Yes	Yes (1 mL HNO_3)	–	Storage in freeze container
Archive samples without acid	–	Plastic	250×2**	Yes	No	–	Storage in freeze container

* Suprapur acid is used for conservation of samples.

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

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
TIMS	Thermal Ionization 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
HCO ₃ ⁻	Alkalinity titration	0.2	1	mg/L	4%	<10%
pH	Pot. Meas.	–	–	–	5%	–
Cond.	Cond. Meas.	0.02	1	mS/m	4%	–
Cl ⁻	Mohr titration	5	70	mg/L	5%	<10%
Cl ⁻	IC	0.2	0.5		6%	10%
SO ₄ ²⁻	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 ⁻	ISE	–	–		–	–
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%
Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainties ²	"Total" uncertainty ³
Fe(II), Fe(tot)	Spectro-photometry	5	20	µg/L	15% (>30 µg/L)	20%
HS ⁻	Spectro-photometry	2	30–200 200–500	µg/L	18% 30 µg/L	20%
NO ₂ -N	Spectro-photometry	–	0.1–20 >20	µg/L	1.1 µg/L 2%	15%
NO ₂ -N +NO ₃ -N	Spectro-photometry	–	0.2–20 >20	µg/L	1.2 µg/L 2.5%	15%
NH ₄ -N	Spectro-photometry	–	0.5–20 >20	µg/L	0.5 µg/L 2.4%	15%
PO ₄ -P	Spectro-photometry	–	0.5–20 >20	µg/L	4.4 µg/L 2.2%	15%
Al, Zn	ICP	–	0.2–0.7	µg/L	12%	20%
Ba, Cr, Mo Pb	ICP	–	0.01–0.3	µg/L	7–10%	20%
Cd, Hg	ICP	–	0.002–0.5	µg/L	5–9%	20%
Co, V	ICP	–	0.005–0.05	µg/L	5–8%	20%
Cu	ICP	–	0.1–0.5	µg/L	8%	20%
Ni	ICP	–	0.05–0.5	µg/L	8%	20%
P	ICP	–	1–40	µg/L	6%	15%
As	ICP	–	0.01–0.5	µg/L	20%	Within the same size (low conc.)

Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainty ²	"Total" uncertainty ³
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Y, Hf	ICP	–	0.005–0.05	µg/L	10%	Within the same size (low conc.)
Sc, In, Th	ICP	–	0.05–0.5	µg/L	10%	Within the same size (low conc.)
Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainties ²	"Total" uncertainty ³
Rb, Zr, Sb, Cs, Tl	ICP	–	0.025–0.25	µg/L	10%	Within the same size (low conc.)
U	ICP	–	0.001–0.01	µg/L	12%	Within the same size (low conc.)
DOC	See Table A10-1	–	0.5	mg/L	8%	30%
TOC	See Table A10-1	–	0.5	mg/L	10%	30%
δ ² H	MS	–	2	‰ SMOW ⁴	1.0 ‰	–
δ 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	–
δ ³⁷ Cl	ICP MS	–	0.2 ‰ (20 mg/L)	‰ SMOC ⁶	–	–
δ 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 ¹³	0.05 Bq/L	Right order of magnitude
²²² Rn, ²²⁶ Ra	LSC	–	0.1	Bq/L	0.05 Bq/L	

- Reporting limits at salinity ≤ 0.4% (520 mS/m) and ≤ 3.5% (3,810 mS/m) respectively.
- Measurement uncertainty reported by consulted laboratory, generally 95% confidence interval.
- Estimated total uncertainty by experience (includes effects of sampling and sample handling).
- Per mill deviation¹¹ from SMOW (Standard Mean Oceanic Water).
- TU=Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of 10⁻¹⁸ (1 Bq/L Tritium = 8.45 TU).
- Per mill deviation¹¹ from SMOC (Standard Mean Oceanic Chloride).
- Per mill deviation¹¹ from PDB (the standard PeeDee Belemnite).
- The following relation is valid between pmC (percent modern carbon) and Carbon-14 age: pmC = 100 × e^{(1950 - y - 1.031)/8274} where y = the year of the C-14 measurement and t = C-14 age
- Per mill deviation¹² from CDT (the standard Canyon Diablo Troilite).
- Isotope ratio without unit.
- The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232:
1 ppm U = 12.4 Bq/kg²³⁸U
1 ppm Th = 3.93 Bq/kg²³²Th
- Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as: δ‰ = 1,000 × (K_{sample} - K_{standard}) / K_{standard}, where K = the isotope ratio and ‰ = ²H, ¹⁸O, ³⁷Cl, ¹³C or ³⁴S etc.

Compilation of water analysis data

Table A10-1. Water Composition.

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	SO4-S mg/L	Br mg/l	F ⁻ mg/L	Si mg/L	Fe mg/L	Fe-tot mg/L	Fe(II) mg/L	Mn mg/L	Li mg/L
KLX17A	416.00	437.51	11763	2007-03-05	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
KLX17A	416.00	437.51	11764	2007-03-06	-	-	-	-	-	192	254	-	-	-	-	-	-	-	-	-	-
KLX17A	416.00	437.51	11765	2007-03-12	1.57	195	2.79	37.3	6.0	183	254	13.7	5.58	0.98	2.83	8.93	2.36	2.37	2.34	0.0833	0.027
KLX17A	416.00	437.51	11766	2007-03-15	0.59	240	3.30	50.4	7.8	169	362	17.0	6.89	1.15	3.31	8.97	1.54	1.48	1.45	0.0831	0.035
KLX17A	416.00	437.51	11767	2007-03-19	-2.56	265	3.52	54.1	8.3	154	450	19.1	7.61	1.56	2.87	8.51	1.09	1.06	1.06	0.0826	0.036
KLX17A	416.00	437.51	11768	3/21/2007	-2.28	276	3.75	57.9	8.5	147	476	20.0	7.86	1.73	2.87	8.55	0.974	0.987	0.956	0.0839	0.038
KLX17A	416.00	437.51	11769	3/23/2007	-3.71	273	3.55	57.1	8.4	142	490	20.6	7.31	1.77	2.84	8.18	0.844	0.907	0.876	0.0819	0.038
KLX17A	416.00	437.51	11770	3/30/2007	2.11	195	2.86	40.2	6.0	165	262	13.3	6.85	0.92	2.77	8.82	1.74	1.70	1.70	0.119	0.027
KLX17A	416.00	437.51	11771	4/2/2007	-0.26	275	3.61	59.0	8.3	140	455	19.4	8.65	1.64	3.05	8.56	1.31	1.22	1.26	0.108	0.037
KLX17A	416.00	437.51	11772	4/4/2007	-1.84	292	3.74	61.4	8.8	136	508	20.8	9.01	1.79	2.73	8.53	1.11	0.980	1.05	0.103	0.040
KLX17A	416.00	437.51	11773	4/11/2007	-	-	-	-	-	126	560	22.4	-	1.98	2.69	-	-	-	-	-	-
KLX17A	416.00	437.51	11809	4/12/2007	-0.93	322	4.01	68.3	9.4	122	565	22.9	9.75	2.00	2.66	8.41	0.791	0.729	0.690	0.0988	0.045
KLX17A	416.00	437.51	11810	4/18/2007	-0.78	329	3.96	67.7	9.6	118	576	24.0	9.09	2.19	2.71	8.18	0.876	0.892	-	0.108	0.046
KLX17A	416.00	437.51	11811	4/18/2007	-	-	-	-	-	118	573	24.3	-	2.24	2.67	-	-	0.888	-	-	-
KLX17A	416.00	437.51	11812	4/23/2007	-1.17	332	3.97	69.2	9.8	115	591	24.4	9.60	2.25	2.68	8.35	0.871	0.761	0.759	0.108	0.054
KLX17A	642.00	701.10	11612	1/31/2007	-	-	-	-	-	114	633	-	-	-	-	-	-	-	-	-	-
KLX17A	642.00	701.10	11635	2/1/2007	-5.81	216	3.37	35.6	4.8	176	340	23.1	7.73	1.20	3.05	8.48	0.667	0.414	0.286	0.0535	0.030
KLX17A	642.00	701.10	11684	2/5/2007	-2.05	91.9	1.29	11.3	2.1	247	20.1	7.13	3.12	<0.2	3.36	7.90	0.348	0.304	0.304	0.0436	0.013
KLX17A	642.00	701.10	11688	2/8/2007	-1.55	91.8	1.32	11.4	2.1	246	19.9	7.06	3.19	<0.2	3.46	8.08	1.35	1.35	1.35	0.0358	0.013
KLX17A	642.00	701.10	11689	2/12/2007	-3.31	89.5	1.21	10.9	2.0	248	19.7	7.10	3.77	<0.2	3.49	7.87	2.07	2.13	2.11	0.0327	0.012
KLX17A	642.00	701.10	11690	2/21/2007	-0.64	91.4	1.38	11.8	2.4	239	19.0	7.10	3.97	<0.2	3.87	8.84	1.36	1.14	1.04	0.0372	0.012
KLX17A	642.00	701.10	11691	2/23/2007	-1.45	88.0	1.33	11.8	2.3	237	16.8	6.81	4.03	<0.2	3.80	8.20	0.875	0.789	0.785	0.0261	0.012
KLX17A	642.00	701.10	11692	2/26/2007	-1.00	88.0	1.30	12.0	2.1	238	17.1	6.47	2.80	<0.2	3.75	6.90	0.740	0.694	0.682	0.0250	<0.05
KLX17A	642.00	701.10	11693	2/26/2007	-	-	-	-	-	238	17.1	6.51	-	<0.2	3.81	-	-	0.690	0.680	-	-
KLX17A	642.00	701.10	11694	2/28/2007	-0.03	90.7	1.48	11.9	2.3	235	18.0	6.23	3.61	<0.2	3.88	9.13	0.324	0.346	0.305	0.0121	0.013

Idcode	Secup	Seclow	Sample	Sr	I ⁻	pH	DOC	TOC	HS ⁻	Drill water	EiCond	NH ₄ -N	NO ₂ -N	NO ₃ -N	NO ₂ ⁻ -N+NO ₃ ⁻ -N	PO ₄ -P	P	Density
	m	m	no.	mg/L	mg/L		mg/L	mg/L	mg/L	%	mS/m	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	g/mL
KLX17A	416.00	437.51	11763	-	-	-	-	-	-	1.16	-	-	-	-	-	-	-	-
KLX17A	416.00	437.51	11764	-	-	8.11	-	-	-	1.31	117	-	-	-	-	-	-	-
KLX17A	416.00	437.51	11765	0.792	0.010	7.78	7.4	7.4	0.016	1.18	119	0.0262	0.0002	0.0013	0.0014	0.0018	0.0090	-
KLX17A	416.00	437.51	11766	1.11	0.012	8.06	4.1	-	0.023	1.51	149	0.0617	0.0002	0.0025	0.0027	0.0040	0.0127	-
KLX17A	416.00	437.51	11767	1.30	0.013	8.07	3.6	3.7	0.019	1.65	169	0.0704	0.0002	0.0005	0.0006	0.0040	0.0062	-
KLX17A	416.00	437.51	11768	1.40	0.013	8.11	3.5	3.7	0.018	1.67	269	0.0623	0.0004	0.0027	0.0031	0.0038	0.0035	-
KLX17A	416.00	437.51	11769	1.37	0.013	8.07	3.5	-	0.025	1.75	183	-	<0.0002	0.0009	0.0010	0.0049	0.0051	-
KLX17A	416.00	437.51	11770	0.846	0.009	7.72	17	-	0.016	0.98	120	0.0323	0.0002	0.0011	0.0014	0.0020	0.0037	-
KLX17A	416.00	437.51	11771	1.40	0.013	7.85	6.2	6.4	0.027	1.60	174	0.0572	0.0002	0.0022	0.0024	0.0018	0.0111	-
KLX17A	416.00	437.51	11772	1.49	0.014	7.92	5.6	-	0.042	1.71	189	0.0448	<0.0002	0.0055	0.0056	0.0023	0.0097	-
KLX17A	416.00	437.51	11773	-	-	7.91	-	-	-	1.72	203	-	-	-	-	-	-	-
KLX17A	416.00	437.51	11809	1.69	0.015	7.96	3.4	3.4	0.028	1.80	217	0.0639	<0.0002	0.0021	0.0022	0.0033	0.0037	-
KLX17A	416.00	437.51	11810	1.69	0.020	7.92	3.7	3.2	0.019	1.71	209	0.0557	0.0002	0.0038	0.0040	0.0028	0.0032	0.9978
KLX17A	416.00	437.51	11811	-	-	7.93	-	-	0.024	1.66	209	0.0541	-	-	-	-	-	-
KLX17A	416.00	437.51	11812	1.72	0.022	7.95	3.3	3.3	0.028	1.72	214	0.0576	<0.0002	0.0062	0.0062	0.0041	0.0057	-
KLX17A	642.00	701.10	11612	-	-	8.24	-	-	-	7.14	225	-	-	-	-	-	-	-
KLX17A	642.00	701.10	11635	0.866	-	8.39	4.6	-	<0.006	3.49	144	0.0561	0.0007	<0.0003	0.0009	0.0041	-	-
KLX17A	642.00	701.10	11684	0.217	0.004	8.46	4.1	4.6	<0.006	0.26	49.6	0.0444	0.0004	0.0004	0.0008	0.0079	0.0127	-
KLX17A	642.00	701.10	11688	0.211	-	8.47	4.3	-	<0.006	0.24	48.2	0.0474	0.0005	0.0004	0.0009	0.0094	-	-
KLX17A	642.00	701.10	11689	0.200	0.004	8.38	4.3	4.8	<0.006	0.23	47.7	0.0576	0.0004	0.0014	0.0018	0.0093	0.0271	-
KLX17A	642.00	701.10	11690	0.206	0.004	8.26	5.1	5.5	<0.006	0.26	47.4	0.0426	0.0006	0.0004	0.0010	0.0074	0.0342	-
KLX17A	642.00	701.10	11691	0.200	-	8.17	5.7	-	<0.006	0.21	45.8	0.0161	0.0004	0.0009	0.0013	0.0082	-	-
KLX17A	642.00	701.10	11692	0.200	0.004	8.36	5.1	4.7	<0.006	0.21	45.7	0.0276	0.0002	0.0005	0.0007	0.0092	0.0172	0.9973
KLX17A	642.00	701.10	11693	-	-	8.33	-	-	<0.006	0.21	45.3	0.0286	-	-	-	-	-	-
KLX17A	642.00	701.10	11694	0.206	0.004	8.22	7.6	-	<0.006	0.23	47.6	0.0298	0.0004	<0.0003	0.0005	0.0144	-	-

- = Not analysed

< "value" = results less than detection limit

ChargeBal % = Rel. charge balance error %

SICADA: water_composition

Table A10-2. Trace Elements.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	U mg/L	Th mg/L	As mg/L	Sc mg/L	Cd mg/L	Hg mg/L	V mg/L	Rb mg/L	Y mg/L	Zr mg/L	In mg/L	Cs mg/L	Ba mg/L	La mg/L
KLX17A	416,00	437,51	11765	2007-03-12	0.132	0.0213	0.170	<0.05	0.0056	0.0420	0.477	5.97	0.0884	0.548	<0.05	0.198	107	0.758
KLX17A	416,00	437,51	11767	2007-03-19	0.128	<0.02	0.160	<0.05	<0.002	0.0560	0.405	7.45	0.0664	0.358	<0.05	0.239	152	0.370
KLX17A	416,00	437,51	11768	2007-03-21	0.123	<0.02	0.170	<0.05	<0.002	0.0499	0.357	7.79	0.0634	0.284	<0.05	0.233	160	0.305
KLX17A	416,00	437,51	11771	2007-04-02	0.114	<0.02	0.110	<0.05	<0.002	0.0099	0.339	7.77	0.0589	0.248	<0.05	0.213	164	0.152
KLX17A	416,00	437,51	11809	2007-04-12	0.116	<0.02	0.100	<0.05	<0.002	0.0286	0.280	9.22	0.0513	0.223	<0.05	0.256	190	0.0675
KLX17A	416,00	437,51	11810	2007-04-18	0.103	<0.02	<0.10	<0.05	0.0073	<0.002	0.333	9.36	0.0563	0.047	<0.05	0.241	202	0.0424
KLX17A	416,00	437,51	11812	2007-04-23	0.101	<0.02	<0.10	<0.05	0.0056	<0.002	0.283	9.31	0.0512	0.046	<0.05	0.239	205	0.0366
KLX17A	642,00	701,10	11684	2007-02-05	0.241	<0.02	0.185	<0.05	0.0069	<0.002	0.619	3.10	0.0572	0.149	<0.05	0.111	31.8	0.110
KLX17A	642,00	701,10	11689	2007-02-12	0.297	<0.02	0.235	<0.05	0.0050	<0.002	0.450	3.29	0.0761	0.173	<0.05	0.141	43.3	0.118
KLX17A	642,00	701,10	11690	2007-02-21	0.271	0.0724	0.178	<0.05	0.0069	<0.002	1.17	3.20	0.1760	0.464	<0.05	0.193	38.6	0.914
KLX17A	642,00	701,10	11692	2007-02-26	0.220	<0.02	0.167	<0.05	0.0094	<0.002	0.522	2.79	0.0721	0.182	<0.05	0.110	27.9	0.126

Table A10-2. Trace Elements. Continued.

Idcode	Secup m	Seclow m	Sample no.	Hf mg/L	Tl mg/L	Ce mg/L	Pr mg/L	Nd mg/L	Sm mg/L	Eu mg/L	Gd mg/L	Tb mg/L	Dy mg/L	Ho mg/L	Er mg/L	Tm mg/L	Yb mg/L	Lu mg/L
KLX17A	416,00	437,51	11765	0.0449	<0.005	0.801	0.0712	0.231	0.0177	<0.005	0.0127	<0.005	0.0089	<0.005	0.0081	<0.005	0.0096	<0.005
KLX17A	416,00	437,51	11767	0.0316	<0.005	0.382	0.0336	0.111	0.0086	<0.005	0.0076	<0.005	0.0059	<0.005	<0.005	<0.005	0.0063	<0.005
KLX17A	416,00	437,51	11768	0.0246	<0.005	0.298	0.0273	0.0860	0.0072	<0.005	0.0062	<0.005	0.0056	<0.005	<0.005	<0.005	0.0055	<0.005
KLX17A	416,00	437,51	11771	0.0192	<0.005	0.163	0.0140	0.0467	<0.005	<0.005	0.0051	<0.005	<0.005	<0.005	<0.005	<0.005	0.0052	<0.005
KLX17A	416,00	437,51	11809	0.0209	<0.005	0.0703	0.0068	0.0247	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
KLX17A	416,00	437,51	11810	<0.005	<0.005	0.0397	<0.005	0.0155	<0.005	0.0230	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
KLX17A	416,00	437,51	11812	<0.005	<0.005	0.0322	<0.005	0.0124	<0.005	0.0234	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005	<0.005
KLX17A	642,00	701,10	11684	<0.005	<0.005	0.161	0.0179	0.0721	0.0102	<0.005	0.0102	<0.005	0.0080	<0.005	0.0065	<0.005	0.0089	<0.005
KLX17A	642,00	701,10	11689	<0.005	<0.005	0.153	0.0171	0.0719	0.0102	<0.005	0.0107	<0.005	0.0094	<0.005	0.0083	<0.005	0.0104	<0.005
KLX17A	642,00	701,10	11690	0.0101	<0.005	1.280	0.130	0.466	0.0578	0.011	0.0433	0.0051	0.0295	0.0059	0.0187	<0.005	0.0163	<0.005
KLX17A	642,00	701,10	11692	<0.005	<0.005	0.182	0.0199	0.0838	0.0114	<0.005	0.0110	<0.005	0.0091	<0.005	0.0076	<0.005	0.0093	<0.005

< "value" = result less than detection limit
 SICADA: trace_elements

Table A10-3. Isotopes I (H-, O-, B-, S-, Cl-, and C-isotopes).

Idcode	Secup m	Seclow m	Sample no	Sampling date	$\delta^2\text{H}$ dev SMOW	^3H TU	$\delta^{18}\text{O}$ dev SMOW	$^{10}\text{B}/^{11}\text{B}$ no unit	$\delta^{34}\text{S}$ dev CDT	$\delta^{13}\text{C}$ dev PDB	$^{87}\text{Sr}/^{86}\text{Sr}$ no unit	^{14}C pmC	$\delta^{37}\text{Cl}$ dev SMOC
KLX17A	416.00	437.51	11764	2007-03-06	-93.1	9.9	-12.5	-	-	-	-	-	-
KLX17A	416.00	437.51	11765	2007-03-12	-93.6	6.2	-12.5	0.2318	28.4	-16.2	0.71527	50.4	-0.37
KLX17A	416.00	437.51	11766	2007-03-15	-100.1	3.0	-13.1	-	-	-	-	-	-
KLX17A	416.00	437.51	11767	2007-03-19	-102.8	2.4	-13.7	0.2329	30.2	-16.8	0.71525	45.0	-0.08
KLX17A	416.00	437.51	11768	2007-03-21	-104.5	2.8	-13.9	0.2327	30.3	-17.0	0.71524	44.2	-0.21
KLX17A	416.00	437.51	11769	2007-03-23	-105.6	2.6	-14.0	-	-	-	-	-	-
KLX17A	416.00	437.51	11770	2007-03-30	-92.4	4.3	-12.3	-	-	-	-	-	-
KLX17A	416.00	437.51	11771	2007-04-02	-103.2	4.6	-13.6	0.2354	30.4	-17.1	0.71524	52.9	-0.05
KLX17A	416.00	437.51	11772	2007-04-04	-107.9	1.5	-14.3	-	-	-	-	-	-
KLX17A	416.00	437.51	11809	2007-04-12	-111.1	0.90	-14.4	0.2321	31.3	-16.8	0.71522	44.3	-0.19
KLX17A	416.00	437.51	11810	2007-04-18	-110.8	1.6	-14.4	0.2384	32.1	-16.4	0.71526	42.6	0.05
KLX17A	416.00	437.51	11812	2007-04-23	110.9	1.3	-14.5	0.2387	31.8	-16.2	0.71519	41.0	0.04
KLX17A	642.00	701.10	11612	2007-01-31	-110.4	<0.8	-14.7	-	-	-	-	-	-
KLX17A	642.00	701.10	11635	2007-02-01	-97.0	4.1	-13.0	-	-	*	-	-	*
KLX17A	642.00	701.10	11684	2007-02-05	-79.4	2.1	-10.9	0.2368	16.2	-16.8	0.71510	50.3	0.05
KLX17A	642.00	701.10	11688	2007-02-08	-79.3	2.4	-10.8	-	-	-	-	-	-
KLX17A	642.00	701.10	11689	2007-02-12	-79.4	32.2	-10.8	0.2368	15.2	-17.0	0.71511	50.5	-0.08
KLX17A	642.00	701.10	11690	2007-02-21	-81.3	3.0	-10.9	0.2364	17.2	-16.7	0.71516	51.8	-0.16
KLX17A	642.00	701.10	11691	2007-02-23	-80.2	2.7	-10.9	-	-	-	-	-	-
KLX17A	642.00	701.10	11692	2007-02-26	-79.6	1.9	-10.9	0.2369	18.6	-16.4	0.71512	52.7	0.16
KLX17A	642.00	701.10	11694	2007-02-28	-79.7	3.4	-10.8	-	-	-	-	-	-

- = Not analysed

< "value" = result less than detection limit

* = sample stored in freezer/refrigerator

SICADA: isotopes_1

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

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 At time of analysis	²²² Rn Bq/L At time of collection
KLX17A	416.00	437.51	11765	2007-03-12	*	*	*	*	*	-	25.1	99.8
KLX17A	416.00	437.51	11767	2007-03-19	*	*	*	*	*	0.10	19.9	28.7
KLX17A	416.00	437.51	11768	2007-03-21	*	*	*	*	*	<0.015	10.8	183
KLX17A	416.00	437.51	11771	2007-04-02	*	*	*	*	*	<0.015	26.6	42.9
KLX17A	416.00	437.51	11810	2007-04-18	1.40	0.18	6.00	0.20	0.30	<0.015	14.0	47.6
KLX17A	416.00	437.51	11811	2007-04-18	*	*	*	*	*	<0.015	12.7	44.4
KLX17A	416.00	437.51	11812	2007-04-23	*	*	*	*	*	<0.015	31.6	60.7
KLX17A	642.00	701.10	11684	2007-02-05	*	*	*	*	*	<0.015	45.4	74.7
KLX17A	642.00	701.10	11689	2007-02-12	*	*	*	*	*	0.022	25.0	40.1
KLX17A	642.00	701.10	11690	2007-02-21	*	*	*	*	*	<0.015	26.4	42.6
KLX17A	642.00	701.10	11692	2007-02-26	2.90	0.18	3.00	0.20	0.30	<0.015	25.4	41.4
KLX17A	642.00	701.10	11693	2007-02-26	*	*	*	*	*	<0.015	22.2	37.1

* = Sample stored in freezer/refrigerator
 < "value" = result less than detection limit
 SICADA: isotopes_2

Table A10-5. Dissolved gases.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Ar mL/L	He mL/L	N ₂ mL/L	CO ₂ mL/L	CH ₄ mL/L	O ₂ mL/L	H ₂ μL/L	CO μL/L	C ₂ H ₆ μL/L	C ₂ H ₄ μL/L	C ₂ H ₂ μL/L	C ₂ H ₂ ⁻⁴	C ₃ H ₈ μL/L	C ₃ H ₆ μL/L	DISS_GAS mL/L H ₂ O
KLX17A	416.00	437.51	11810	2007-04-18	0.77	0.18	65	0.71	0.070	0.028	<2.0	<3.3	0.28	0.21	<0.05	–	0.07	0.07	67.4
KLX17A	642.00	701.10	11692	2007-02-28	0.35	<0.0021	64.6	1.34	0.145	0	0.7	1.35	0.12	–	–	0.030	<0.05	<0.05	66.4

< "value" = result below detection limit
 SICADA: gas_dissolved