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Oskarshamn site investigation

Hydrogeochemical analyses in percussion boreholes in Simpevarp and Laxemar in 2003, 2005 and 2006

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December 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.

Data in SKB's database can be changed for different reasons. Minor changes in SKB's database will not necessarily result in a revised report. Data revisions may also be presented as supplements, available at www.skb.se.

A pdf version of this document can be downloaded from www.skb.se.

Abstract

This report summarises results from water sampling in connection with hydraulic tests and tracer tests in 15 percussion boreholes within the site investigation programme at Oskarshamn site investigation area: HLX20, HLX21, HLX23, HLX27, HLX28, HLX30, HLX32, HLX33, HLX34, HLX37, HLX38, HLX39, HLX42, HLX43 and HSH02.

The results from this activity include groundwater chemistry data in accordance with SKB chemistry classes 1, 3 and 5. Data from HSH02 (located at Simpevarp subarea) were obtained during August 2003 and all other data (from Laxemar subarea) were obtained during 2005 and 2006.

All analytical data from the activity are stored in the SICADA database.

Sammanfattning

Denna rapport sammanfattar resultat från vattenprovtagning i samband med hydrauliska tester och spårförsök i 15 hammarborrhål; HLX20, HLX21, HLX23, HLX27, HLX28, HLX30, HLX32, HLX33, HLX34, HLX37, HLX38, HLX39, HLX42, HLX43 och HSH02 inom platsundersökningen i Oskarshamn.

Resultaten från denna aktivitet inkluderar vattenkemidata enligt SKB kemiklass 1, 3 och 5. Proverna från HSH02 (belägen i delområde Simpevarp) är tagna under augusti 2003 och alla andra prov (från delområde Laxemar) är tagna under 2005 och 2006.

Alla resultat från vattenanalyserna finns i SKB:s databas SICADA.

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1 Introduction

This document reports data collected from hydraulic tests and tracer tests in percussion boreholes during 2003, 2005 and 2006. These activities are part of the site investigation at Oskarshamn /1–3/. Controlling documents for performing this activity are listed in Table 1-1. The activity plans as well as the method description are SKB internal controlling documents. The field work is reported in the database SICADA, traceable using the activity plan number.

The activity includes water sampling (handling routines and analytical methods are reported in Appendix 1) from boreholes according to SKB chemistry class 1, 3 and 5 (see Table 1-2). Archive samples from some of the sampling occasions were stored in a freezer (Appendix 2).

A map showing the locations of the percussion boreholes within the investigation site at Oskarshamn is presented in Figure 1-1.

Activity plan	Number	Version
Hydrotester och vattenprover i hammarborrhål HSH02 och rymda delen i kärnborrhål KSH03	AP PS 400-03-046	1.0
Interferenstester i HLX34 och HLX35	AP PS 400-05-034	1.0
Hydrauliska tester i HLX10, HLX21–HLX33	AP PS 400-04-105	1.0
Interferenstester i HLX36 och HLX37	AP PS 400-05-069	1.0
Flödesloggning i HLX21, HLX35 och HLX38	AP PS 400-06-014	1.0
Interferens och spårämnenstester mellan HLX33 och SSM228 och SSM229	AP PS 400-06-036	1.0
Interferenstest mellan HLX39 och HLX40, HLX41 samt KLX17A 0–65,45 m	AP PS 400-06-102	1.0
Flödesloggning med HTHB i i HLX14, HLX18, HLX20, HLX27, HLX28, HLX32, HLX33, HLX37 och HLX39	AP PS 400-06-110	1.0
Hammarborrning av HLX42 med tillägg	AP PS 400-06-109	1.0
Method description	Number	Version
Enkel vattenprovtagning i hammarborrhål och kärnborrhål	SKB MD 423.002	1.0

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

Borehole	Borehole length (m)	SKB chemistry class
HLX20	9.03–202.20	3*
HLX21	9.03-150.30	3**/5***
HLX23	6.03-160.20	3**
HLX27	6.03–164.70	3*
HLX28	6.03–154.20	3*
HLX30	9.03–163.40	3**
HLX32	12.30-162.60	3*
HLX33	9.03-202.10	5/3*
HLX34	9.00–151.80	3**
HLX37	12.03-199.80	3**/3*/5
HLX38	15.10–199.50	3**
HLX39	6.00–199.30	5/3*
HLX42	9.10-152.60	1
HLX43	6.00-170.60	3*
HSH02	12.00–200.00	3****

Table 1–2. Borehole ID, borehole length and SKB chemistry class.

* No analysis of major cations.

** Including options of $\delta^2 H,~\delta^{18} O,~^{13} C,~^{14} C$ (pmC), $^{34} S,~^{87} Sr,~\delta^{37} Cl,~^{10} B/^{11} B,~^{3} H$ and TOC.

*** Excluding $\delta^2 H,\,{}^3H,\,\delta^{18}O,\,I^-\!,\,HS^-\!,\,NH_4,\,NO_2\text{+}NO_3$ and $PO_4.$

**** Including options of $\delta^2 H,\,\delta^{18} O,\,\delta^{37} C I,\,{}^{10} B/{}^{11} B,\,{}^{3} H$ and TOC.

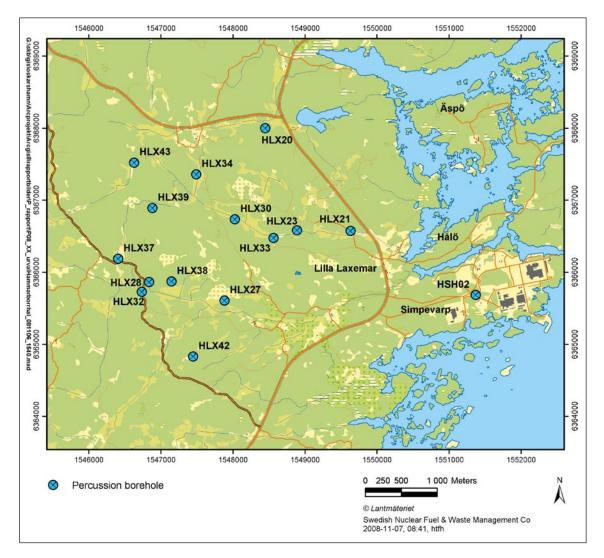


Figure 1-1. Overview of the Oskarshamn site investigation area, showing the sampled percussion boreholes.

2 Objective and scope

This report summarises results from the water samples collected in connection with hydraulic tests and tracer tests in 15 percussion boreholes within the site investigation programme at Oskarshamn /1,2/: HLX20, HLX21, HLX23, HLX27, HLX28, HLX30, HLX32, HLX33, HLX34, HLX37, HLX38, HLX39, HLX42, HLX43 and HSH02. The purpose of the sampling was to investigate the areal distribution of the water composition as well as to obtain information about the chemistry in shallow groundwater. The chemistry sampling has been conducted in connection with hydraulic tests and tracer tests. Further information about other borehole activities can be found in the various P-reports /4–12/.

3 Equipment and methods

3.1 HTHB used for water sampling in HLX20, HLX21, HLX27, HLX28, HLX32, HLX33, HLX37, HLX38, HLX39, HLX43 and HSH02

3.1.1 Overview

The basic equipment used in these tests is called HTHB (Swedish abbreviation for Hydraulic Test System for Percussion Boreholes). The use and function of this equipment is described in the report from the flow logging in HSH02 /12/.

The HTHB unit is designed to perform pumping and hydraulic injection tests in open percussion drilled boreholes (Figure 3-1), as well as in isolated borehole sections (Figure 3-2), down to a total depth (borehole length) of 200 m. With the HTHB unit, it is also possible to perform flow logging along the borehole during open-hole pumping tests (Figure 3-1). For injection tests, the upper packer cannot be located deeper than c. 80 m due to limitations of the equipment.

All equipment that belongs to the HTHB system is, when not in use, stored on a trailer and can easily be transported by a standard car. The equipment includes a submersible borehole pump with housing, expandable packers, pressure sensors and a pipe string and/or hose. During flow logging, sensors measuring temperature, electric conductivity and down-hole flow rate are employed as well. The total flow rate at the surface of the borehole is manually adjusted by a control valve and monitored using an electromagnetic flow meter. A data logger samples data at a frequency determined by the operator.

The packers are normally expanded using pressurized water unless the groundwater level is low or if the risk of freezing makes the use of water unsuitable. In such cases, the packers are expanded using nitrogen gas. A folding container is used to collect and store the discharged water from the borehole for subsequent use in injection tests (if required).

3.1.2 Test performance

The main pumping test is normally preceded by a shorter capacity test to determine a suitable pumping flow rate. During the capacity test, the flow rate may be adjusted according to the obtained response. Usually the main pumping is carried out as a single-hole constant flow rate test followed by a pressure recovery period, but it can also be performed as a constant pressure (or flow) injection test. The entire pump test usually lasts for approximately ten hours to ensure steady-state conditions.

Before flow logging of the borehole starts, the intention is to achieve approximately steady-state conditions in the borehole. The flow logging is performed with the flow logging probe lifted (injection test) or lowered (pumping test) at a velocity of 1-3 m/min. A more detailed description of flow logging is presented in /12/.

During a normal test, three water samples are taken. The first sample is taken after about one hour of pumping, the second after four hours and the last just before pump stop. These water samples are taken from a valve located after the flow meter (see Figure 3-1).

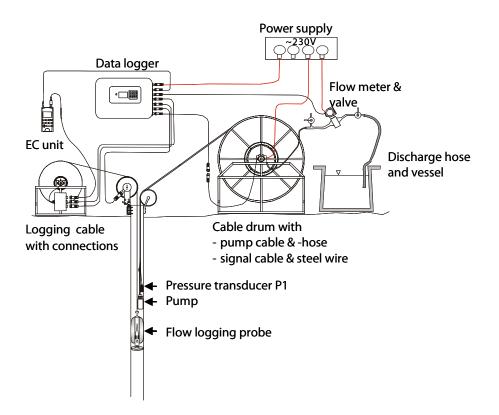


Figure 3–1. Schematic test set–up for a pumping test in an open borehole in combination with flow logging with HTHB. (From SKB MD 326.001, SKB internal document).

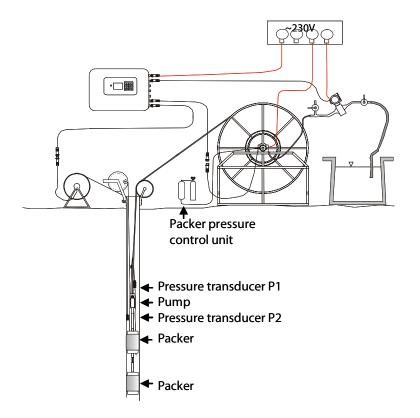


Figure 3–2. Schematic test set–up for a pumping test in an isolated borehole section with HTHB. (From SKB MD 326.001, SKB internal document).

3.2 Water sampling during hydraulic interference tests

3.2.1 Water sampling in boreholes HLX30, HLX33, HLX34, HLX37, HLX39 and HLX42

The pumping and interference tests in these boreholes have been performed with an integrated field unit at the pumped borehole, Figure 3-3, consisting of a container housing. In the borehole the following equipment is installed;

- Submersible pump: Grundfos SPE5-70, range is about 5–100 L/min.
- Absolute pressure transducer: Druck PTX1830, 10 bar range and $\pm 0.1\%$ accuracy.
- Water level dipper.
- Flow gauge: Krohne IFM1010 electromagnetic, 0–150 L/min.

The submersible pump is usually connected to a PEM hose and then installed at a depth of 40 to 80 metres of depth. In addition, a pressure gauge and also often a PEM-hose used for the level dipper is lowered to the same depth. The pumped water passes the flow meter and a regulating unit at the surface and is then discharged. The water samples are usually taken at the discharge point or from a valve located after the flow meter and regulating unit.

Data from on-line monitoring of the discharged water parameters were stored in two different logging units (CR10 and CR23). The data from the loggers were downloaded either continuously (CR10 and CR23) or by disk to the DMS database.

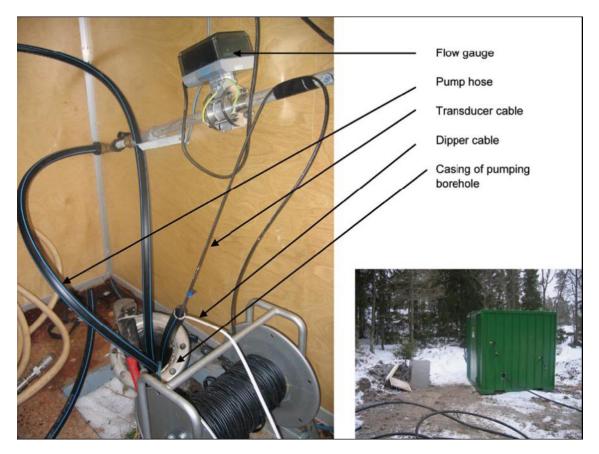


Figure 3–3. Container for the test equipment (right) and instrumentation (left) in borehole.

3.2.2 Water sampling in boreholes HLX21 and HLX23

During the interference tests in HLX21 and HLX23, slightly different test equipment was used as follows:

- Submersible pump, Grundfos MS 402 SP2A-23.
- Integrated logger/absolute transducer MiniTroll Advance (In-Situ Inc.), measurement range 0-300 PSIA.
- Light- and sound water level indicator (dipper).

Apart from this, the system is the same as described in the preceding section.

3.2.3 Water sampling in borehole HLX42

Water sampling (SKB sample no. 11529) for HLX42 was performed during the last day of drilling and the sampled water was pumped from the entire length of the borehole. Hence the water was pumped with the drilling equipment and analysed only for EC.

4 Execution

4.1 General

The activities were performed in accordance with corresponding Activity Plans (Table 1-1), and following the method description SKB MD 423.002 (Enkel vattenprovtagning i hammarborrhål och kärnborrhål, SKB internal controlling document). The pumping periods are shown in Table 4-1 and the sampling procedures and analytical methods are reported in Appendix 1.

4.2 Handling of water analysis data

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

Some of the constituents are determined by more than one method and/or laboratory. 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.
- Calculation of charge balance errors, equation (1). Relative errors within ± 5% are considered acceptable.

Relative error (%) =
$$100 \times \frac{\sum \text{cations(equivalents)} - \sum \text{anions(equivalents)}}{\sum \text{cations(equivalents)} + \sum \text{anions(equivalents)}}$$
 (1)

• General 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 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 4-1.

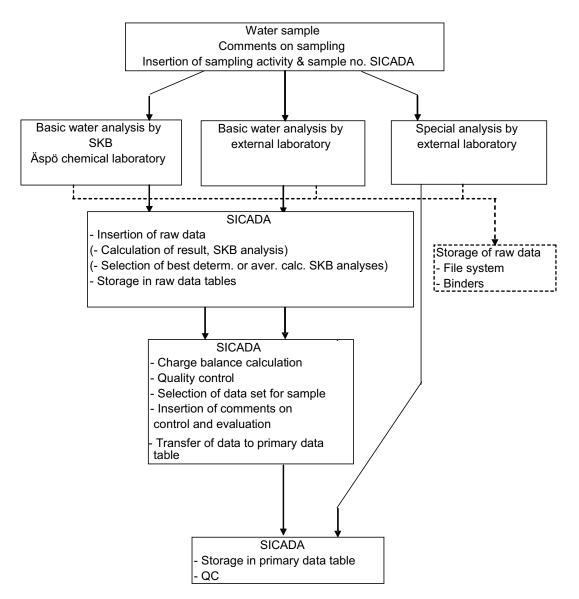


Figure 4-1. Overview of data management for hydrogeochemical data.

4.3 Water sampling, sample treatment and analyses

The pumped water from the borehole section was conveyed from the pipe into a 25 L container. Filtration, conservation and portioning of the water samples into sample flasks were performed indoors following transport from the site to the laboratory. A water sample is defined as ground-water collected at one occasion and consists of several sample portions, labelled with the same sample number.

The pumping periods in connection with sampling are reported in Table 4-1. An overview of sample handling routines and analytical methods is given in Appendix 1. The routines are applicable independently of sampling method or type of sampling object.

Borehole	Section [m]	Start date and time	Stop date and time	Sampling date and time	SKB sample no.
HLX20	9.03–202.2	2006-11-10 09:08	2006-11-10 15:06	2006-11-10 13:21	11508
HLX21	9.00–150.3	2005-08-15 13:15	2005-08-19 12:25	2005-08-15 14:15	10451
HLX21	9.03–150.3	2005-08-15 13:15	2005-08-19 12:25	2005-08-19 12:22	10458
HLX21	9.03–150.3	2006-05-18 12:26	2006-05-18 21:21	2006-05-18 14:30	11072
HLX23	6.03–160.20	2005-06-28 10:32	2005-07-01 11:45	2005-06-28 11:32	10394
HLX23	6.03–160.20	2005-06-28 10:32	2005-07-01 11:45	2005-07-01 11:41	10402
HLX27	6.03–164.70	2006-11-24 09:07	2006-11-24 14:40	2006-11-24 14:40	11557
HLX28	6.03–154.20	2006-11-08 10:51	2006-11-08 15:59	2006-11-08 15:57	11504
HLX30	9.03–163.40	2005-09-02 13:25	2005-09-09 09:31	2005-09-05 14:25	10487
HLX30	9.03–163.40	2005-09-02 13:25	2005-09-09 09:31	2005-09-09 09:25	10495
HLX32	12.30–162.60	2006-11-30 12:11	2006-11-30 15:51	2006-11-30 15:56	11567
HLX33	9.03–202.10	2006-06-28 14:38	2006-08-07 15:19	2006-06-29 07:40	11206
HLX33	9.03–202.10	2006-11-12 09:06	2006-11-12 14:24	2006-11-12 14:20	11512
HLX34	9.00–151.80	2005-06-16 12:20	2005-06-20 07:10	2005-06-16 14:20	10362
HLX34	9.00–151.80	2005-06-16 12:20	2005-06-20 08:10	2005-06-20 08:08	10371
HLX37	12.03–199.80	2005-10-18 11:34	2005-10-24 11:06	2005-10-18 12:51	10542
HLX37	12.03–199.80	2005-10-18 11:34	2005-10-24 11:06	2005-10-21 08:40	10561
HLX37	12.03–199.80	2005-11-10 10:46	2005-11-10 14:03	2005-11-10 14:01	10608
HLX37	12.03–199.80	2006-11-02 08:49	2006-11-02 14:38	2006-11-02 14:37	11497
HLX38	15.10–199.50	2006-05-22 12:46	2006-05-22 22:30	2006-05-22 22:15	11078
HLX39	6.00–199.30	2006-09-01 10:20	2006-09-02 10:58	2006-09-01 12:40	11305
HLX39	6.10–199.30	2006-11-06 08:55	2006-11-06 16:03	2006-11-06 15:50	11502
HLX42	9.10–152.60	2006-11-13 13:30	2006-11-16 19:00	2006-11-16 14:20	11529
HLX43	6.00–170.60	2006-12-02 09:27	2006-12-02 18:42	2006-12-02 14:25	11573
HSH02	12.00–200.00	2003-08-27 09:03	2003-08-27 20:01	2003-08-27 10:30	5802
HSH02	12.00–200.00	2003-08-27 09:03	2003-08-27 20:01	2003-08-27 15:20	5803
HSH02	12.00–200.00	2003-08-27 09:03	2003-08-27 20:01	2003-08-27 19:30	5804

Table 4-1. Pumping periods in the sampled boreholes.	Table 4-1.	Pumping	periods in	the sampled	boreholes.
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The archive samples have been stored in a freezer container at Äspö or in freezer storage in Oskarshamn. The location and dates for storage of archive samples are listed in Appendix 2.

Note: The freezer for sample flasks had thawed on 2008-02-28, which means that seven of the archive samples; from HLX21 (SKB no 10451, 10458), HLX30 (SKB no 10487, 10495), and HLX37 (SKB no 10451, 10458) stored in connection with the groundwater sampling have been affected (SKB Dok id 1168893; SKB internal meeting record). The reason for this was lack of power combined with a malfunction of the alarm.

5 Results

The results comprise water chemistry data from sampling in borehole HLX20, HLX21, HLX23, HLX27, HLX28, HLX30, HLX32, HLX33, HLX34, HLX37, HLX38, HLX39, HLX42, HLX43 and HSH02. The results from the chemical analyses are presented below and in Appendix 3.

Original data from the reported activity are stored in the primary database SICADA and data are traceable in SICADA by the Activity Plan number (Table 1-1). Only data in SICADA database are accepted for further interpretation and modelling. The data presented in this report are regarded as copies of the original ones. Data in the SICADA database may be revised if needed. However, such revision of the SICADA 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.

5.1 Basic water analyses

The basic water analyses include Na, K, Ca, Mg, Fe, Si, Li, Mn, S, Sr, SO_4^{2-} , Cl⁻, Si, HCO_3^{-} , Br⁻, F⁻, I⁻, HS⁻, NH₄⁺, NO₂⁻, NO₃⁻, TOC and DOC. Furthermore, measurements are made of pH, electrical conductivity and density. The basic water analysis data and relative charge balance errors are compiled in Appendix 3, Table A3-1. The charge balance error gives an indication of the quality and uncertainty of the analyses of major constituents. The charge balance error did not exceed the acceptable level of \pm 5% in any case.

Sulphate (SO_4^{2-}) analysed using ion chromatography (IC) is compared with sulphate determined as total sulphur using inductively coupled plasma atomic emission spectrometry (ICP-AES) and presented in Figure 5-1. Sulphur generally exists as sulphate species and the discrepancies are within the analysis error.

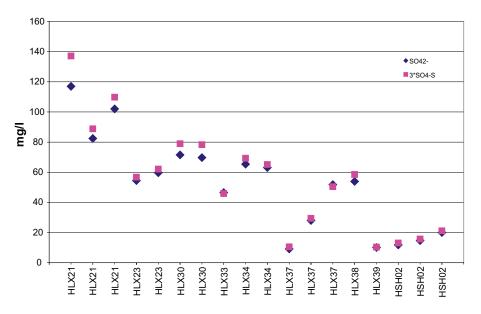


Figure 5–1. Sulphate (SO₄^{2–} by IC) data compared to sulphate calculated from total sulphur ($3xSO_4$ –S by ICP) data from samples collected in the investigated sections.

The chloride concentrations are plotted versus the corresponding electric conductivity values in Figure 5-2. The plot gives an approximate indication that the values are reasonable. The data from the borehole sections agree well with earlier data from the Äspö Hard Rock Laboratory.

5.2 Stable and radioactive isotopes

The isotope determinations include the stable isotopes δ^2 H, δ^{18} O, 10 B/ 11 B, δ^{34} S, δ^{13} C δ^{37} Cl and 87 Sr/ 86 Sr as well as the radioactive isotopes 3 H (TU) and 14 C (pmC). The isotope data are compiled in Appendix 3, Table A3-2. The 3 H and δ^{18} O results are presented in Figure 5-3. The 3 H content was below the detection limit (0.8 Tritium Units (TU)) in HLX30 and HLX34. The highest amounts of were found in HSH02, located near the Oskarshamn nuclear power plant.

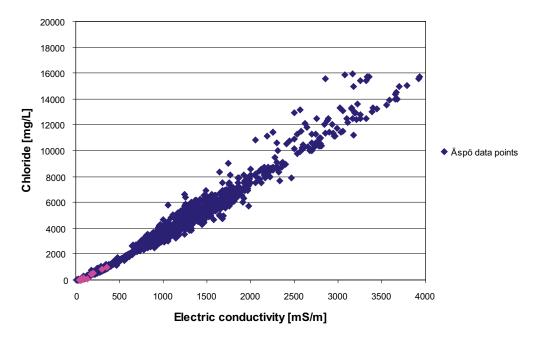


Figure 5–2. Chloride concentration versus electrical conductivity. Data points from the reported water samples are shown as pink rhombi.

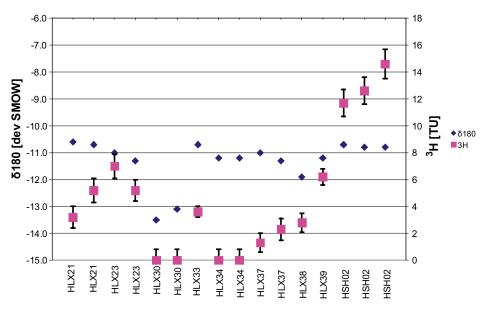


Figure 5–3. $\delta^{18}O$ and ³*H* data from samples collected in the investigated boreholes.

6 Summary

- A comparison of the results from different laboratories and/or methods showed satisfactory agreement.
- The charge balance error did not exceed the acceptable level of \pm 5% in any of the analysed samples.
- General judgement of plausibility based on earlier results and experience indicated reasonable values.

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Appendix 1

Sampling and analytical methods

Table A1-1.	Sample handling	routines and	analytical	methods.

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within - or delivery time to lab.
Drill water	Uranine	Plastic (brown)	100	No	No	Spectrofluorometry	-
Anions	HCO₃ ⁻ 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 ⁻ , SO₄ ²⁻ , Br⁻, F⁻) ISE (F⁻)	Not critical (month)
	Br (control sample to external laboratory)	Plastic	100	Yes	No	ICP MS	Not critical (month)
	ŀ	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 HCI)	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	Frozen, transported in isolated bag	Spectrophotometry	Short transportation time
	NH ₄ -N	Glass (measuring flask)	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)

Component group	Component/ element	Sample container	Volume	Filtering	Preparation/	Analysis method	Analysis within - or
		(material)	(mL)		Conservation*		delivery time to lab.
Dissolved organic Carbon	DOC	Plastic	250	Yes	Frozen, transported in isolated bag	UV oxidation, IR	Short transportation time
Total organic Carbon	TOC	Plastic	250	No	Frozen, transported in isolated bag	UV oxidation, IR	Short transportation time
Environmental isotopes	δ²Η, δ¹8Ο	Plastic	100	No	-	MS	Not critical (month)
Tritium	³ H (enhanced.)	Plastic (dry bottle)	500	No	_	LSC	Not critical (month)
Chlorine-37	δ³²CI	Plastic	500	No	_	ICP MS	Not critical (month)
Carbon isotopes	δ ¹³ C, pmC (¹⁴ C)	FLPE	125×2	No	-	(A)MS	A few days
Sulphur isotopes	δ ³⁴ S	Plastic	1000	No	_	Combustion, ICP MS	No limit
Strontium-isotopes	⁸⁷ Sr/ ⁸⁶ Sr	Plastic	100	No	_	TIMS	Days or Week
Uranium and Thorium isotopes	²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th,	HDPE	1000	No	-	Chemical separat. Alfa/gamma spectrometry	No limit
Boron isotopes	¹⁰ B/ ¹¹ B	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP MS	No limit
Radon and Radium isotopes	²²² Rn, ²²⁶ Ra	HDPE	1000	No	No	LSC	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

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within - or delivery time to lab.
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

IR Infra Red detection

MS Mass Spectrometry

LSC Liquid Scintillation Counting

(A)MS (Accelerator) Mass Spectrometry

TIMS Thermal Ionization Mass Spectrometry

GC Gas Chromatography

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
HCO ₃ -	Alkalinity titration	1	mg/L	4%
рН	Potentiometric	3–10	pH unit	±0.10 pH units
Cond.	Electrical Conductivity Meas.	1–150 150–10 000	mS/m	5% 3%
CI-CI-	Mohr titration IC	≥70 0.5–70	mg/L	5% 8%
SO4 ²⁻	IC	0.5	mg/L	12%
Br− Br⁻	IC ICP SFMS	DL 0.2, RL 0.5 0.001, 0.004, 0.010⁴	mg/L	15% 25%
F- F-	IC ISE	DL 0.2, RL 0.5 DL 0.1, RL 0.2	mg/L	13% 12%
-	ICP SFMS	0.001, 0.004, 0.0104	mg/L	25% ⁵
Na	ICP AES	0.1	mg/L	13%
К	ICP AES	0.4	mg/L	12%
Са	ICP AES	0.1	mg/L	12%
Mg	ICP AES	0.09	mg/L	12%
S(tot)	ICP AES	0.16	mg/L	12%
Si(tot)	ICP AES	0.03	mg/L	14%
Sr	ICP AES	0.002	mg/L	12%
Li	ICP AES	4	µg/L	12%
Fe	ICP AES	0.02	mg/L	13.3%6
Fe	ICP SFMS	$0.0004, 0.002, 0.004^4$	µg/L	20% ⁶
Mn	ICP AES	0.003	µg/L	12%5
Mn	ICP SFMS	0.00003, 0.00004, 0.00014	mg/L	53% ⁶
Fe(II), Fe(tot)	Spectrophotometry	DL 0.006, RL 0.02	µg/L	0.005 (0.02–0.05 mg/L) 9% (0.05–1 mg/L) 7% (1–3 mg/L)
HS⁻	Spectrophotometry	DL 0.006, RL 0.02	µg/L	25%
NO ₂ -N	Spectrophotometry	0.1	µg/L	2%
NO ₂ -N +NO ₃ -N	Spectrophotometry	0.2	µg/L	0.2 (0.2–20μg/L) 2%(> 20 μg/L)
NH4-N	Spectrophotometry	11	µg/L	30% (11–20 µg/L) 25% (20–50 µg/L) 12% (50–1 200 µg/L)
PO ₄ -P	Spectrophotometry	0.7	µg/L	0.7 (0.7–20μg/L) 3% (> 20 μg/L)
AI	ICP SFMS	0.2, 0.3, 0.74	µg/L	18% ⁶
Zn	ICP SFMS	0.2, 0.8, 24	µg/L	16, 18, 26% ⁶
Ba, Cr, Mo	ICP SFMS	0.01, 0.04, 0.14	µg/L	Ba 15%⁴, Cr 22%⁵ Mo 39%⁵
Pb	ICP SFMS	0.01, 0.1, 0.34	µg/L	15% ⁶
Cd	ICP SFMS	0.002, 0.02, 0.54	µg/L	16% ⁶
Hg	ICP AFS	0.002	µg/L	11% ⁶
Со	ICP SFMS	0.005, 0.02, 0.054	µg/L	26% ⁶
V	ICP SFMS	0.005, 0.03, 0.054	µg/L	18%6
Cu	ICP SFMS	0.1, 0.2, 0.54	µg/L	14%6
Ni	ICP SFMS	0.05, 0.2, 0.54	µg/L	16% ⁶
Р	ICP SFMS	1, 5, 404	µg/L	16%6
As	ICP SFMS	0.01 (520 mS/m)	µg/L	59% ⁶
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu	ICP SFMS	0.005, 0.02, 0.054	µg/L	20%, 20%, 25% ⁶

Table A1-2. Rep	porting limits and measure	ement uncertainties (u	pdated in 2008).

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
Sc, In, Th	ICP SFMS	0.05, 0.2, 0.54	µg/L	25% ⁶
Rb, Zr, Sb, Cs	ICP SFMS	0.025, 0.1, 0.254	µg/L	15%, 20%, 20%⁵, 25% ⁶
ТІ	ICP SFMS	0.025, 0.1, 0.254	µg/L	14% ^{5,6}
Y, Hf	ICP SFMS	0.005, 0.02, 0.054	µg/L	15%, 20%, 20% ⁵ , 25% ⁶
U	ICP SFMS	0.001, 0.005, 0.014	µg/L	14%, 16%⁵, 19%, 18%, 21% ⁶
DOC	UV oxidation, IR Carbon analysator	0.5	mg/L	8%
ТОС	UV oxidation, IR Carbon analysator	0.5	mg/L	10%
$\delta^2 H$	MS	2	‰ SMOW ⁸	0.9 (one standard dev.)
δ ¹⁸ Ο	MS	0.1	‰ SMOW ⁸	0.1 (one standard dev.)
³Н	LSC	0.8	TU ⁹	0.8 TU
δ ³⁷ Cl	ICP MS	0.2	‰ SMOC ¹⁰	0.217
$\delta^{13}C$	A (MS)	_	‰ PDB ¹¹	0.317
pmC (14C)	A (MS)	-	pmC ¹²	0.417
δ ³⁴ S	MS	0.2	‰ CDT ¹³	0.4 (one standard dev.)
⁸⁷ Sr/ ⁸⁶ Sr	TIMS	-	No unit (ratio) ¹⁴	0.00002
¹⁰ B/ ¹¹ B	ICP SFMS	-	No unit (ratio) ¹⁰	-
²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th	Alfa spectr.	0.0001	Bq/L ¹⁵	≤5% (Counting statistics uncertainty)
²²² Rn, ²²⁶ Ra	LSC	0.015	Bq/L	≤5% (Counting statistics uncertainty)

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

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

- 3. Measurement uncertainty reported by the laboratory, generally as ± percent of measured value in question at 95% confidence interval.
- 4. Reporting limits at electrical cond. 520 mS/m, 1440 mS/m and 3810 mS/m respectively.
- 5. Measurement uncertainty at concentrations 100×RL.
- 6. Measurement uncertainty at concentrations 10×RL.
- 7 Determined only in surface waters. PON, POP and POC refers to Particulate Organic Nitrogen, Phosphorous and Carbon, respectively.
- 8. Per mille deviation from SMOW (Standard Mean Oceanic Water).
- 9. TU=Tritium Units, where one TU corresponds to a tritium/hydrogen ratio of 10⁻¹⁸ (1 Bq/L Tritium = 8.45 TU).
- 10. Per mille deviation from SMOC (Standard Mean Oceanic Chloride).
- 11. Per mille deviation from PDB (the standard PeeDee Belemnite).
- 12. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age: pmC = 100 x e^{((1950-y-1.03t)/8274)} where y = the year of the C-14 measurement and t = C-14 age.
- 13. Per mille deviation from CDT (the standard Canyon Diablo Troilite).
- 14. 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.
- 16. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as: $\delta^{y}I = 1000 \times (K_{sample}-K_{standard})/K_{standard}$, where K= the isotope ratio and ${}^{y}I = {}^{2}H$, ${}^{18}O$, ${}^{37}CI$, ${}^{13}C$ or ${}^{34}S$ etc.
- 17. SKB estimation from duplicate analyses by the contracted laboratory.

Appendix 2

Archive samples

		Main components	B10 Env. Met. Lant. Trace el.		Deut	Deut			C13		Archive 250 ml	Freezer storage	Sent for analysis	Final Freezer storage
SKB no	Date			тос	O18	Sr87	Trit.	CI-37	pmC	S34	(no)	(date, sign)		(date, sign)
10362	050616		1		1	1	1	1	2	1		050616/HH	Sent	
10362	050616										2	050616/HH		070126/HH
10371	050620		1		1	1	1	1	2	1		050620/HH	Sent	
10371	050620										2	050620/HH		070126/HH
10394	050628		1		1	1	1	1	2	1		050628/HH	Sent	
10394	050628										2	050628/HH		070126/HH
10402	050701		1		1	1	1	1	2	1		050701/HH	Sent	
10402	050701										2	050701/HH		070126/HH
10451	050815		1		1	1	1	1	2	1		050815/UJ		
10451	050815										2	050815/UJ		
10458	050819		1		1	1	1	1	2	1		050819/UJ		
10458	050819										2	050819/UJ		
10487	050905		Х		Х	Х	Х	х	2	Х		050905/HH		
10487	050905										2	050905/HH		
10495	050909		х		Х	Х	Х	х	2	Х		050909/HH		
10495	050909										2	050909/HH		
10542	051018		х		Х	Х	Х	х	2	Х		051018/HH		
10542	051018										2	051018/HH		
10561	051021		х		Х	Х	х	Х	2	Х		051021/HH		
10561	051021										2	051021/HH		
10608	051110		х	Х	Х	Х	Х	х	2	Х		051110/HH		
10608	051110										2	051110/HH		
11072	060518	Х	х	Х	Х	Х	Х	х	2	Х		060518/HH		
11072	060518										2	060518/HH		070126/HH
11078	060522	Х	х	Х	Х	Х	Х	х	2	Х		060522/HH		
11078	060522										2	060522/HH		070126/HH
11206	060629	Х	х	Х	х	Х	х	х	2	Х		060629/HH	All sent except C-13, pmC 070507/HH	
11206	060629										2	060629/HH		070223/HH
11305	060901	Х	х	Х	Х	Х	х	Х	2	Х		060901/HH	070314/HH	
11305	060901										2	060901/HH		070126/HH

Appendix 3

Compilation of water analysis data

Table A3-1. Water composition.

ldcode	Secup m	Seclow m	Sample no.	Sampling date and time	Charge Bal %	Na mg/L	K mg/L	Ca mg/L	Mg mg/L	HCO₃⁻ mg/L	CI⁻ mg/L	SO₄²- mg/L	SO₄-S mg/L	Br⁻ mg/l	F⁻ mg/L
HLX20	9.03	202.20	11508	2006-11-10 13:21	_	_	_	_	_	199	53.6	43.5	_	0.23	4.54
HLX21	9.03	150.30	10451	2005-08-15 14:15	4.56	231	4.86	15.9	4.5	250	112	117	45.7	-	4.63
HLX21	9.03	150.30	10458	2005-08-19 12:22	2.65	172	3.82	11.5	3.1	235	72.5	82	29.6	<0.20	4.47
HLX21	0.00	150.30	11072	2006-05-18 14:30	-0.27	182	3.65	12.9	3.6	238	90.6	102	36.6	<0.20	5.05
HLX23	0.00	160.20	10394	2005-06-28 11:32	-1.17	119	4.53	12.9	4.5	221	51.5	55	18.9	<0.20	4.07
HLX23	0.00	160.20	10402	2005-07-01 11:41	-3.09	123	4.11	12.9	3.6	224	56.9	59.7	20.7	<0.20	4.57
HLX27	6.01	164.70	11557	2006-11-24 14:40	-	_	-	-	_	175	1,010	92.0	_	4.16	2.56
HLX28	6.03	154.20	11504	2006-11-08 15:57	_	_	-	_	_	229	88.7	69	_	0.33	4.57
HLX30	0.00	163.40	10487	2005-09-05 14:25	1.69	357	4.29	62.3	8.7	146	520	71.5	26.3	-	2.82
HLX30	0.00	163.40	10495	2005-09-09 09:25	2.68	327	4.17	54.5	7.5	178	428	70	26.1	-	3.05
HLX32	12.30	162.60	11567	2006-11-30 15:56	_	_	_	-	_	260	96.2	81.9	_	0.27	4.45
HLX33	9.03	202.10	11206	2006-06-29 07:40	0.03	167	2.35	15.2	4.4	222	128	46.5	15.3	0.44	4.56
HLX33	9.03	202.10	11512	2006-11-12 14:20	-	_	-	-	-	219	137	44	-	0.53	4.26
HLX34	0.00	151.80	10362	2005-06-16 14:20	-0.54	151	4.12	14.8	4.0	297	44.4	65	23.1	<0.20	5.20
HLX34	0.00	151.80	10371	2005-06-20 08:08	-1.62	146	3.75	15.3	4.0	299	45.1	63	21.7	<0.20	5.03
HLX37	12.03	199.80	10542	2005-10-18 12:51	-0.51	92.8	2.54	10	2.4	248	12.8	9	3.5	<0.20	4.14
HLX37	12.03	199.80	10561	2005-10-21 08:40	0.01	121	2.48	11.6	2.8	226	56.3	28	9.81	<0.20	4.49
HLX37	12.03	199.80	10608	2005-11-10 14:01	1.61	156	3.01	15	3.7	201	109	51.8	16.8	0.33	4.69
HLX37	12.10	199.80	11497	2006-11-02 14:37	-	_	-	-	-	247	14.3	12	-	<0.20	3.69
HLX38	15.02	199.50	11078	2006-05-22 22:15	0.23	471	8.65	111	25.3	194	839	54	19.5	4.18	2.58
HLX39	6.02	199.30	11305	2006-09-01 12:40	-1.43	46.7	2.64	39.8	6.4	226	26.4	10	3.45	<0.20	1.75
HLX39	6.10	199.30	11502	2006-11-06 15:50	-	_	-	-	-	270	81.9	6.1	-	0.30	4.73
HLX42	9.10	152.60	11529	2006-11-16 14:20	-	_	-	-	-	-	_	-	-	-	_
HLX43	6.00	170.60	11573	2006-12-02 14:25	-	-	-	-	-	321	81.8	30	-	0.35	3.93
HSH02	0.00	200.00	5802	2003-08-27 10:30	-0.16	102	3.27	8.6	2.9	285	7.0	12	4.35	<0.20	1.36
HSH02	0.00	200.00	5803	2003-08-27 15:20	0.12	103	2.62	7.4	2.4	268	10.5	15	5.24	<0.20	1.83
HSH02	0.00	200.00	5804	2003-08-27 19:30	-0.07	111	2.48	7.3	2.3	263	21.0	20	7.04	<0.20	2.18

ldcode	Secup m	Seclow m	Sample no.	Sampling date and time	Si mg/L	Fe mg/L	Mn mg/L	Li mg/L	Sr mg/L	рН	TOC mg/L	ElCond mS/m	Density g/mL
HLX20	9.03	202.20	11508	2006-11-10 13:21	_	_	_	_	_	8.27	_	67.6	0.9973
HLX21	9.03	150.30	10451	2005-08-15 14:15	4.71	0.134	0.0530	0.023	0.274	8.28	_	128	0.9965
HLX21	9.03	150.30	10458	2005-08-19 12:22	6.15	0.0636	0.0387	0.018	0.191	8.28	_	84.8	0.9963
HLX21	0.00	150.30	11072	2006-05-18 14:30	6.22	0.0916	0.0452	0.017	0.197	8.24	4.4	92.0	0.9975
HLX23	0.00	160.20	10394	2005-06-28 11:32	12.2	3.59	0.164	0.015	0.126	7.47	-	69.0	0.9964
HLX23	0.00	160.20	10402	2005-07-01 11:41	7.00	1.04	0.126	0.011	0.108	7.60	_	70.4	0.9963
HLX27	6.01	164.70	11557	2006-11-24 14:40	_	-	-	-	-	7.91	_	358	0.9985
HLX28	6.03	154.20	11504	2006-11-08 15:57	_	-	-	-	-	8.06	_	86.9	-
HLX30	0.00	163.40	10487	2005-09-05 14:25	6.26	0.0631	0.0701	0.056	1.24	8.03	_	202	0.9968
HLX30	0.00	163.40	10495	2005-09-09 09:25	6.34	0.0663	0.0630	0.052	1.10	8.09	_	177	0.9967
HLX32	12.30	162.60	11567	2006-11-30 15:56	_	-	-	-	-	8.46	_	87.3	0.9974
HLX33	9.03	202.10	11206	2006-06-29 07:40	6.40	0.0719	0.0394	0.020	0.283	8.28	4.2	87.2	0.9974
HLX33	9.03	202.10	11512	2006-11-12 14:20	_	-	-	-	-	8.18	_	87.7	0.9975
HLX34	0.00	151.80	10362	2005-06-16 14:20	6.38	0.313	0.0578	0.015	0.294	8.26	-	75.6	0.9963
HLX34	0.00	151.80	10371	2005-06-20 08:08	6.22	0.0589	0.0655	0.014	0.297	8.19	_	77.2	0.9963
HLX37	12.03	199.80	10542	2005-10-18 12:51	7.87	0.0880	0.0591	0.011	0.124	8.22	-	45.3	0.9963
HLX37	12.03	199.80	10561	2005-10-21 08:40	7.67	0.0541	0.0554	0.012	0.154	8.22	_	62.5	0.9962
HLX37	12.03	199.80	10608	2005-11-10 14:01	6.79	0.0400	0.0645	0.012	0.209	8.23	3.0	81.6	0.9963
HLX37	12.10	199.80	11497	2006-11-02 14:37	_	_	-	-	-	8.13	_	46.0	0.9978
HLX38	15.02	199.50	11078	2006-05-22 22:15	6.22	0.181	0.210	0.039	1.89	7.96	3.5	302	0.9982
HLX39	6.02	199.30	11305	2006-09-01 12:40	7.65	0.084	0.0915	0.008	0.310	7.79	4.1	45.6	0.9971
HLX39	6.10	199.30	11502	2006-11-06 15:50	_	-	-	-	-	8.14	_	70.3	0.9978
HLX42	9.10	152.60	11529	2006-11-16 14:20	_	-	-	-	-		-	36.4	_
HLX43	6.00	170.60	11573	2006-12-02 14:25	_	-	-	-	-	7.77	-	81.9	0.9975
HSH02	0.00	200.00	5802	2003-08-27 10:30	6.07	0.440	0.0719	0.012	0.087	8.22	9.0	49.6	_
HSH02	0.00	200.00	5803	2003-08-27 15:20	6.07	0.489	0.0509	0.013	0.083	8.31	8.2	50.0	_
HSH02	0.00	200.00	5804	2003-08-27 19:30	6.01	0.437	0.0420	0.012	0.087	8.33	7.4	69.7	_

– = Not analysed.
 < "value" = Result less than detection limit.
 ChargeBal % = Rel. charge balance error %.
 SICADA: "p_water_chemistry".

ldcode	Secup m	Seclow m	Sample no.	Sampling date and time	δ²Η dev SMOW	³H TU	δ ¹⁸ Ο dev SMOW	¹⁰ B/ ¹¹ B no unit	δ³⁴S dev CDT	δ¹³C dev PDB	⁸⁷ Sr/ ⁸⁶ Sr no unit	¹⁴C pmC	δ³7CI dev SMOC
HLX21	9.03	150.30	10451	2005-08-15 14:15	-77.5	3.2	-10.6	0.2380	25.9	-13.36	0.715864	42.07	-0.11
HLX21	9.03	150.30	10458	2005-08-19 12:22	-78.2	5.2	-10.7	0.2390	26.4	-14.92	0.715892	46.44	0.14
HLX23	0.00	160.20	10394	2005-06-28 11:32	-76.5	7.0	-11.0	0.2369	22.6	-16.81	0.715195	57.91	0.06
HLX23	0.00	160.20	10402	2005-07-01 11:41	-76.2	5.2	-11.3	0.2363	23.3	-16.39	0.715244	54.54	0.13
HLX30	0.00	163.40	10487	2005-09-05 14:25	-99.9	<0.8	-13.5	0.2393	18.2	-13.44	0.715475	34.11	0.09
HLX30	0.00	163.40	10495	2005-09-09 09:25	-95.4	<0.8	-13.1	0.2396	21.3	-14.99	0.715453	38.16	-0.02
HLX33	9.03	202.10	11206	2006-06-29 07:40	-81.3	3.6	-10.7	0.2369	24.2		0.715123		0.07
HLX34	0.00	151.80	10362	2005-06-16 14:20	-77.7	<0.8	-11.2	0.2362	29.7	-16.50	0.715821	42.55	0.07
HLX34	0.00	151.80	10371	2005-06-20 08:08	-78.3	<0.8	-11.2	0.2367	30.0	-16.51	0.715824	42.46	0.10
HLX37	12.03	199.80	10542	2005-10-18 12:51	-79.9	1.3	-11.0	0.2383	35.4	-16.02	0.716223	44.13	0.20
HLX37	12.03	199.80	10561	2005-10-21 08:40	-80.7	2.3	-11.3	0.2429	24.2	-15.41	0.715944	40.54	-0.02
HLX38	15.02	199.50	11078	2006-05-22 22:15	-87.4	2.8	-11.9	0.2384	23.7	-14.78	0.715499	51.05	0.14
HLX39	6.02	199.30	11305	2006-09-01 12:40	-82.3	6.2	-11.2	0.2356	12.4	-17.40	0.717363	63.30	0.25
HSH02	0.00	200.00	5802	2003-08-27 10:30	-78.6	11.7	-10.7	0.2407	-	_	-	-	-0.18
HSH02	0.00	200.00	5803	2003-08-27 15:20	-78.6	12.6	-10.8	0.2404	-	_	-	_	-0.16
HSH02	0.00	200.00	5804	2003-08-27 19:30	-78.1	14.6	-10.8	0.2406	_	-	-	-	-0.21

Table A3-2. Isotopes I (H-, O-, B-, S-, C-, Sr- and CI-isotopes).

– = Not analysed.
 < "value" = result less than detection limit.
 SICADA: "p_water_chemistry".