P-06-231

Forsmark site investigation

Sampling and analyses of groundwater from percussion drilled boreholes

Results from the boreholes HFM14, HFM23, HFM24, HFM25, HFM26, HFM27, HFM28, HFM29, HFM30, HFM32, HFM33, HFM34 and HFM35

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December 2006

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Keywords: Forsmark, Percussion borehole, Groundwater, Chemical analyses, Isotope determination, Water sampling, AP PF 400-05-121, AP PF 400-06-036, AP PF 400-06-037.

Abstract

Percussion boreholes are drilled as monitoring wells or as flushing water supply wells for core drilling. Further, percussion boreholes are drilled for general geological characterisation or in order to investigate specific geological features (e.g. lineaments) down to about 200 m depth in the bedrock.

Groundwater samples were collected in connection with hydraulic pumping tests in the percussion drilled boreholes HFM14, HFM23–30 and HFM32–35. The analytical protocol included major constituents and isotope options (δD, δ^{18}O, ^{10}B/^{11}B and Tritium) according to SKB class 3. The main objective was to gain hydrogeochemical data to approximately 200 m depth from a number of boreholes spread within the candidate area. Water samples were collected at three occasions during the pumping period. Boreholes HFM14, HFM23, HFM24, HFM26 and HFM35 show increasing chloride concentrations during the pumping period while the other boreholes demonstrate either stable or somewhat varying chloride concentrations.

The analytical results obtained are consistent and the relative charge balance error does not exceed 5% in any of the samples.

Sammanfattning

Hammarborrhål borras dels för att övervaka grundvattennivåförändringar, dels för att utgöra spolvattenbrunnar vid kärnborrning. Vidare används hammarborrhål för allmän geologisk karakterisering och för att undersöka specifika geologiska företeelser (t ex lineament) ner till ca 200 m djup i berggrunden.

Grundvattenprov hart tagits ut under hydrauliska pumptester från hammarborrhålen HFM14, HFM23–30 och HFM32–35. Analysomfattningen inkluderade huvudkomponenter och isotoptillvalen δD, δ^{18}O, ^{10}B/^{11}B och tritium enligt SKB klass 3. Syftet med aktiviteten var att erhålla hydrogeokemiska data ner till ca 200 m djup från flera borrhål spridda inom kandidatområdet. Vattenprover togs vid tre tidpunkter under pumpningen. Hammarborrhålen HFM14, HFM23, HFM24, HFM26 och HFM35 visar ökande kloridkoncentrationer under pumpperioden medan övriga undersökta borrhål mätte stabila eller något varierande kloridhalter.

Analysresultaten är konsistenta och det relativa felet i jonbalansen överskrider inte 5 % för något av proven.

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1 Introduction

This document reports the performance and the results of the activity "Sampling of percussion boreholes after drilling", which is one of the activities performed within the site investigation at Forsmark /1/. The work was carried out in accordance with the activity plans AP PF 400-05-121, AP PF 400-05-125, AP PF 400-06-036 and AP PF 400-06-037. In Table 1-1 controlling documents for conducting this activity are listed. Both activity plans and method descriptions are SKB's internal controlling documents. The report presents hydrogeochemical data from the percussion boreholes HFM14, HFM23–30 and HFM32–35. The length of the boreholes varies between 130 and 210 m /2, 3, 4, 5/.

The locations of the percussion boreholes are shown in Figure 1-1.

Samplings of the boreholes were accomplished in connection with pumping tests and flow logging carried out within the programme for hydrogeological investigations /6, 7, 8, 9, 10, 11, 12/.

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

Activity plan	Number	Version
Hydrotester och vattenprovtagning i hammarborrhålen HFM23, HFM24, HFM25, HFM26, HFM27, HFM28 och HFM32	AP PF 400-05-121	1.0
Provpumpning i borrhål KFM05A (0–114 m) samt Flödesloggning i borrhål HFM14	AP PF 400-05-125	1.0
Hydrotester och vattenprovtagning i hammarborrhålen HFM29, HFM30, HFM31	AP PF 400-06-036	1.0
Hydrotester och vattenprovtagning i hammarborrhålen HFM33, HFM34, HFM35	AP PF 400-06-037	1.0
Method description	**Number**	**Version**
Enkel vattenprovtagning i hammarborrhål och kärnborrhål	SKB MD 423.002	2.0

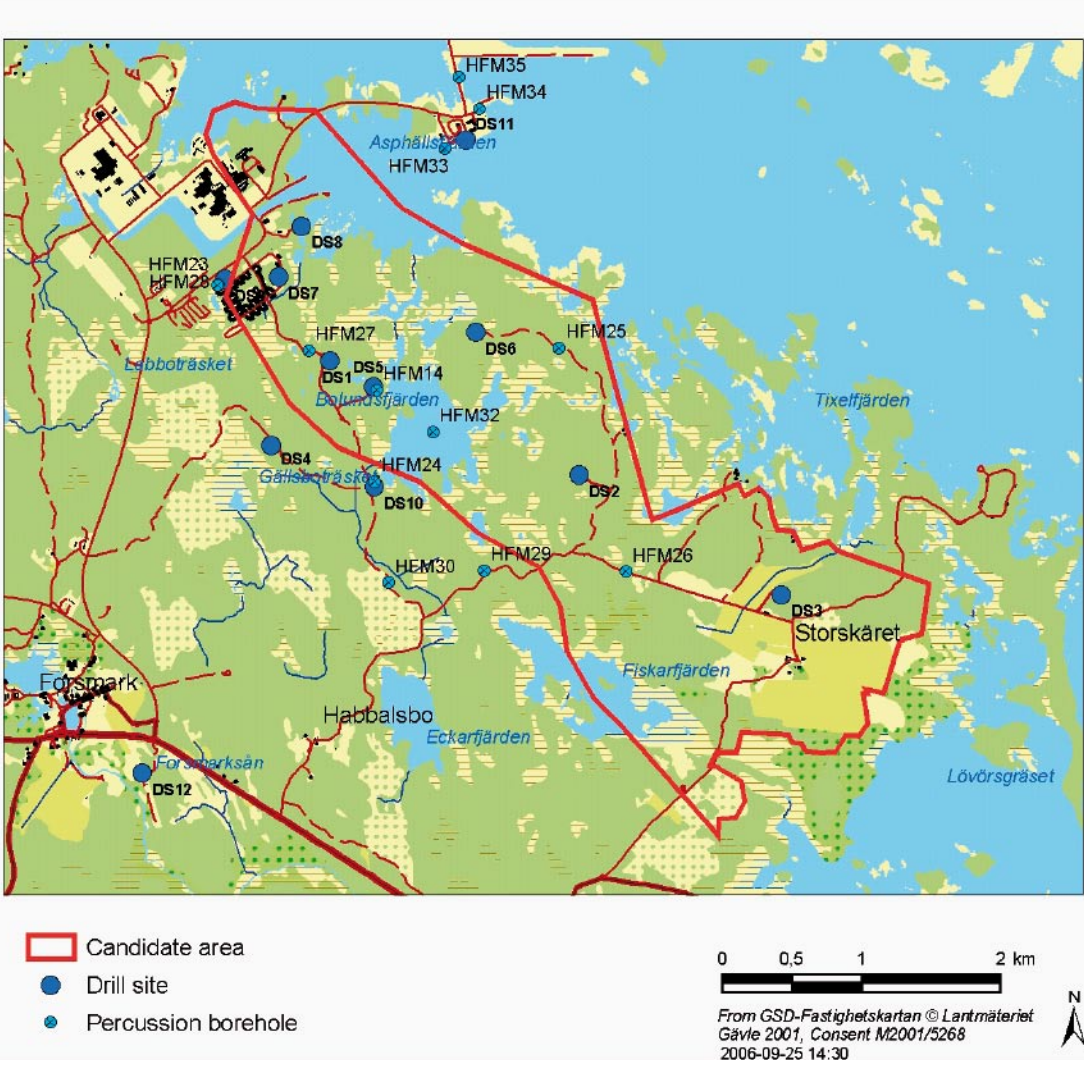

Figure 1-1. *Locations of the investigated boreholes and the drill sites (DS) within the Forsmark investigation area (the area of the map).*

2 Objective and scope

Sampling and analysis of groundwater from the percussion boreholes were mainly performed in order to:

- Gain data on the chemical composition of so called “first strike” groundwater, i.e. groundwater sampled before the impact of short circuiting between fractures of different hydrogeochemical character has become significant.
- Contribute to area coverage of the hydrochemical data from the shallow part of the bedrock.
- Determine the suitability of some of the percussion boreholes to serve as supply wells for the flushing water needed for drilling the cored part of telescopic boreholes. Core drilling of a 1,000 m long borehole consumes approximately 1,000 m^3 water. Core drilled boreholes of SKB chemical-type are of special importance and the total organic content in the flushing water must be low (< 5 mg/L) in order to avoid disturbing the microbiological conditions in the borehole.

Sampling and analysis are performed according to the SKB class 3 procedure. The analyses of the last collected sample from each borehole also include isotope options.

3 Background

The percussion borehole HFM14 was drilled in order to serve as supply well of flushing water for the drilling of KFM05A. The HTHB-tests (pumping test and flow logging) were planned to be conducted in November 2003 /6/ but due to an instable section of the borehole wall at the time, these tests were delayed. The borehole wall has now been stabilised with a longer casing and the tests were performed in April 2006.

The percussion boreholes HFM23 and HFM28 were drilled in the north-western part of the investigation area. Both boreholes were originally planned to be used as flushing water wells for the drilling of KFM09A and KFM09B but the water yield was too low for this purpose. Borehole HFM24 yielded enough water to serve as flushing water well for the core drilling of KFM10A.

Percussion boreholes HFM25, HFM26 and HFM27 were drilled to investigate lineaments, as were the boreholes HFM29 and HFM30.

Borehole HFM32 was drilled on an island in Lake Bolundsfjärden in order to investigate hydrogeological conditions below the lake. Unexpectedly high salinities (4,000 mg/L) have previously been measured in groundwaters from a few soil pipes driven into the lake sediments and this observation needed an explanation.

Percussion boreholes HFM33, HFM34 and HFM35 are all drilled around the SFR facility outside the investigation area. Borehole HFM33 will serve as flushing water well for the core drilling of KFM11A and boreholes HFM34 and HFM35 will be used for pressure monitoring during drilling.

General information concerning the boreholes is presented in Table 3-1.

Table 3-1. Borehole information for HFM14, HFM23–30 and HFM32–35 (from SICADA).

Idcode	Date of completion	Bearing (degrees)	Inclination (degrees)	Northing (m)	Easting (m)	Elevation (m.a.s.l.)	Length (m)
HFM14	2003-10-09	331.7	–59.8	6,699,313,	1,631,734	3.91	150.50
HFM23	2005-09-01	324.3	–58.5	6,700,068	1,630,595	4.25	211.50
HFM24	2005-11-22	47.2	–59.6	6,698,662	1,631,720	3.68	151.35
HFM25	2005-09-08	140.8	–57.8	6,699,616	1,633,039	3.86	187.50
HFM26	2005-11-18	112.4	–53.8	6,698,009	1,633,516	2.73	202.70
HFM27	2005-11-10	337.3	–67.8	6,699,595	1,631,245	2.45	127.50
HFM28	2005-09-14	146.8	–84.8	6,700,068	1,630,597	4.27	151.20
HFM29	2005-12-19	30.0	–58.6	6,698,019	1,632,503	4.47	199.70
HFM30	2006-05-11	28.8	–55.5	6,697,932	1,631,820	0.66	200.75
HFM32	2006-01-14	116.1	–86.1	6,699,015	1,632,137	0.97	202.65
HFM33	2006-05-03	220.0	–59.0	6,701,041	1,632,222	0.05	140.20
HFM34	2006-06-02	30.5	–58.6	6,701,325	1,632,471	2.45	200.75
HFM35	2006-06-14	33.0	–59.2	6,701,557	1,632,321	1.90	200.75

4 Equipment

The sampling in the percussion boreholes was performed in connection with hydraulic tests with the HTHB (Swedish abbreviation for Hydraulic Test System for Percussion Boreholes) and is described in the user manual of the measurement system, SKB internal controlling document SKB MD 326.001 (Mätsystembeskrivning för hydrotestutrustning för hammarborrhål – HTHB). The equipment allows pumping from packed off sections in boreholes of diameter 165 mm and 140 mm (± a few millimetres) using a single- or double packer system. The in-hole equipment includes a packer system, a measurement tube, an enclosed pump, and a combined pressure sensor and data logger. An overview of the HTHB equipment is given in Figure 4-1 and Figure 4-2 below.

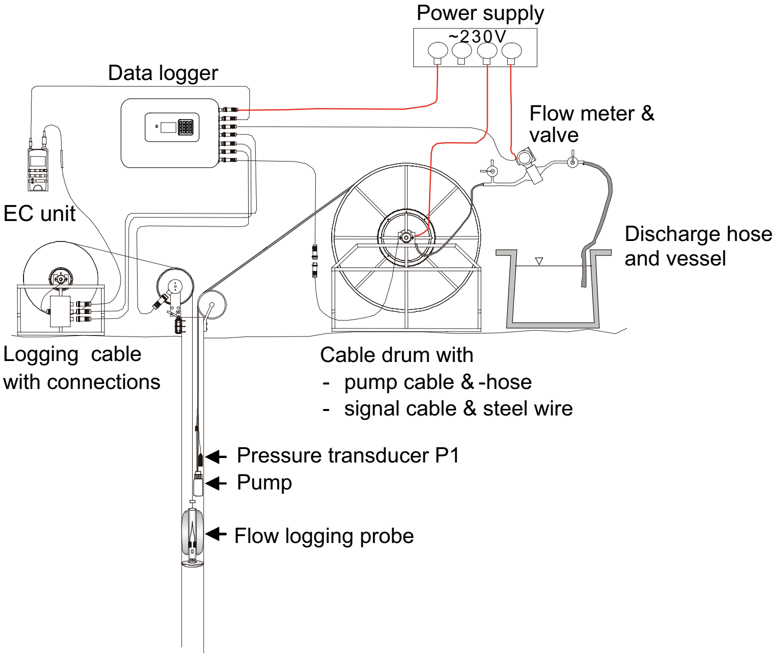

***Figure 4-1.** Schematic test set-up for a pumping test in an open borehole in combination with flow logging with HTHB. (From SKB MD 326.001, SKB internal document).*

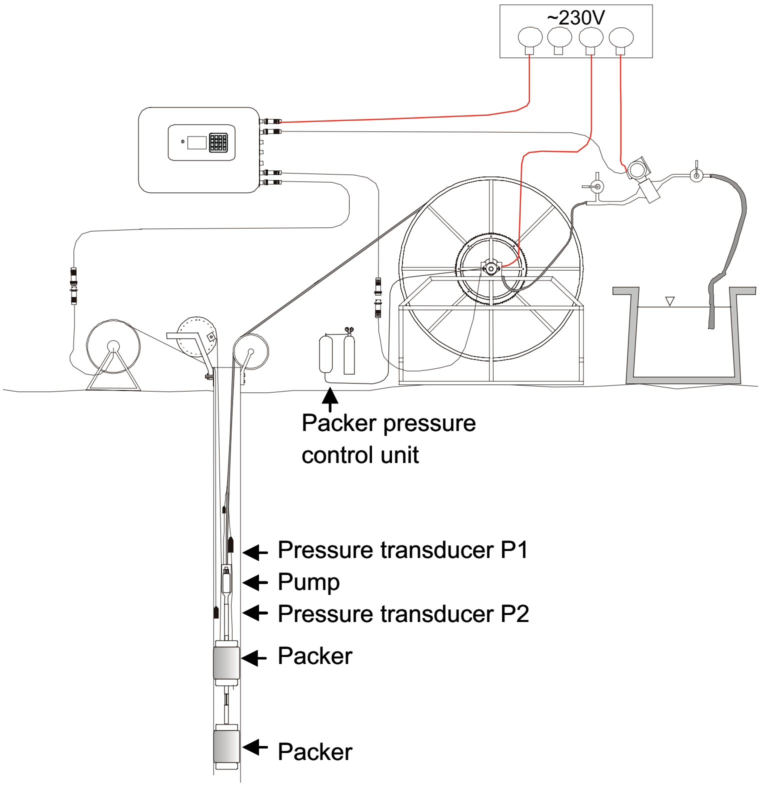

Figure 4-2. *Schematic test set-up for a pumping test in an isolated borehole section with HTHB. (From SKB MD 326.001, SKB internal document).*

5 Execution

5.1 Sampling

Sampling of the percussion boreholes was carried out according to activity plans AP PF 400-05-121, AP PF 400-05-125, AP PF 400-06-037 and AP PF 400-06-037 (SKB internal controlling documents) following the method described in SKB MD 423.002 (Mätsystem – beskrivning för hydrotestutrustning för hammarborrhål – HTHB, SKB internal controlling document)

Generally, the pumping proceeded during 10 hours, and samples were collected three times during the pumping period. Table 5-1 presents general sampling information from the pumping tests.

Table 5-1. Pumping information and collected samples.

Borehole	Pumped section (m)	Date and time of pump start	Date and time of pump stop	Date and time of sampling	Pumped volume (m^3)	Sample no.
HFM14	6.0–150.5	060404 09:31	060404 20:06	060404 09:42	0.8	12220
				060404 16:00	26.5	12219
				060404 20:00	43.25	12221
HFM23	20.8–211.5	060320 09:12	060320 19:12	060320 10:10	0.6	12054
				060320 14:00	3.0	12053
				060320 19:00	5.9	12050
HFM24	18.0–151.4	060207 07:39	060207 18:49	060207 08:45	4.20	12065
				060207 12:25	17.9	12064
				060207 18:45	42.6	12059
HFM25	9.1–187.5	060301 10:32	060301 10:41	060301 10:35	0.61*	12058
HFM26	12.0–202.7	060209 10:10	060209 20:24	060209 11:17	0.56	12056
				060209 15:20	2.73	12055
				060209 20:24	5.48	12049
HFM27	12.0–127.5	060306 10:18	060306 20:25	060306 11:05	2.3	12061
				060306 15:13	14.7	12060
				060306 20:15	29.8	12057
HFM28	12.1–151.2	060315 08:16	060315 18:16	060315 09:17	0.3	12052
				060315 13:16	1.5	12037
				060315 17:50	3.0	12051
HFM29	9.0–199.7	060515 13:37	060515 17:35	060515 15:10	0.4	12255
				060515 17:20	0.5	12257
HFM30	18.0–200.8	060517 09:10	060517 20:15	060517 10:05	3.6	12256
				060517 14:04	18.4	12258
				060517 20:04	38.1	12259
HFM32	5.9–202.7	060117 07:56	060117 18:09	060117 09:40	7.10	12035
				060117 14:02	22.4	12034
				060117 18:00	37.7	12036
	50.0–202.7	060118 14:00	060118 15:30	060118 15:20	1.20	12066

Borehole	Pumped section (m)	Date and time of pump start	Date and time of pump stop	Date and time of sampling	Pumped volume (m^3)	Sample no.
HFM33	12.0–140.2	060509 06:29	060509 16:30	060509 07:52	4.0	12245
				060509 11:55	15.8	12246
				060509 15:55	27.5	12247
HFM34	12.0–200.8	060608 08:07	060608 18:08	060608 08:44	2.50	12289
				060608 11:55	15.7	12290
				060608 17:15	37.9	12291
HFM35	12.0–200.8	060704 09:39	060704 20:03	060704 10:40	2.40	12327
				060704 14:57	12.8	12328
				060704 20:01	25.2	12329

* 0.56 m^3 was pumped out during a capacity test the day before water sampling.

Sampling and analyses were performed according to SKB class 3, but isotope options were included only for the last sample collected from each borehole. Total organic carbon (TOC) was mainly determined in order to investigate the suitability of the boreholes as sources for flushing water.

5.2 Sample treatment and chemical analyses

An overview of sample treatment and analysis routines is given in Appendix 1. The routines are applicable independent of sampling method or type of sampling object.

5.3 Data handling

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

Several components are determined by more than one method and/or laboratory. Moreover, duplicate analyses by an independent laboratory are performed as a standard procedure on each fifth or tenth collected sample.

All analytical results are stored in the SICADA database. The applied hierarchy path "Hydrochemistry/Hydrochemical investigation/Analyses/Water in the database" contains two types of tables, raw data tables and primary data tables (final data tables).

Data on basic water analyses are inserted into 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. Relative errors within ± 5% are considered acceptable (in surface waters ± 10%).

$$rel.\,error\,(\%) = 100 \times \frac{\sum cation\,(equivalent\ s) - \sum anions\,(equivalent\ s)}{\sum cation\,(equivalent\ s) + \sum anion\,(equivalent\ s)}$$

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

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 5-1.

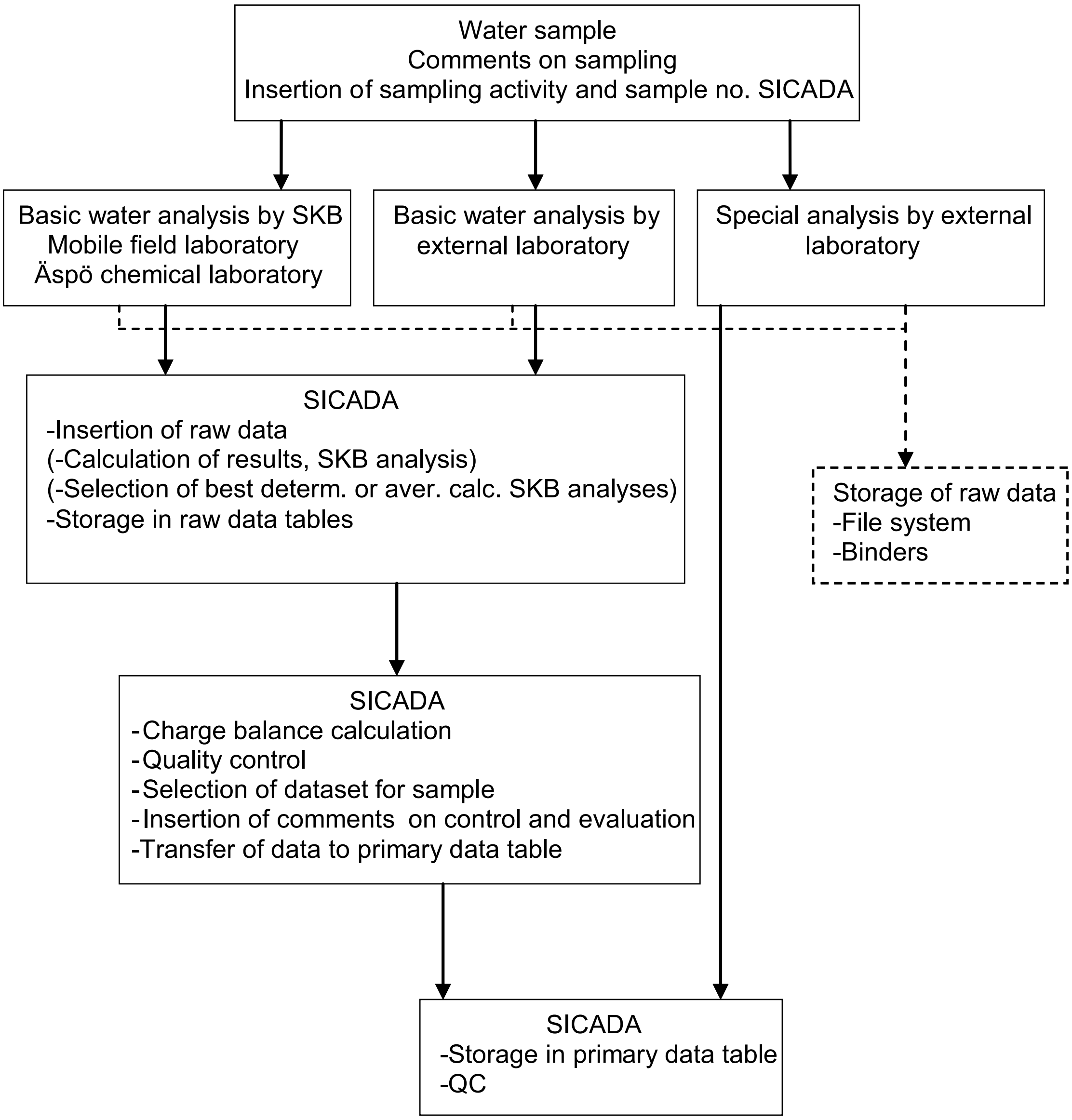

Figure 5-1. *Overview of data management for hydrogeochemical data.*

5.4 Nonconformities

According to SKB MD 423.002 (Vattenprovtagning i hammarborrhål efter borrning, SKB internal controlling document) and /1/, the sampling of groundwater was planned to take place immediately after completion of each percussion borehole. Due to logistic problems this has very seldom been possible. The main problem has been a tight schedule for the different tests in the boreholes. Further, the HTHB equipment has not always been available, and no other suitable equipment exists for pumping and sampling of groundwater in percussion boreholes.

In HFM25 the water yield was found to be very low and therefore only one sample was collected. The sample was taken during a complementary pumping performed immediately after the recovery measurements were finished.

6 Results

6.1 Basic water analysis

The basic water analyses include the major components Na, K, Ca, Mg, S, SO_4^{2-}, Cl^-, Si and HCO_3^- as well as the minor constituents Li, Br, F and TOC (Total Organic Carbon). Furthermore, measurements of pH and electric conductivity are included. The basic water analysis data and relative charge balance errors are compiled in Appendix 2, Table A2-1.

Samples were collected three times in each borehole (except for HFM25 and HFM29); 1) when borehole water reaches the surface, 2) in the middle and 3) in the end of the pumping period. Chloride concentrations from all boreholes and all samples are compared in Figure 6-1. Boreholes HFM14, HFM23, HFM24, HFM26 and HFM35 show a minor increase in the chloride concentration during the pumping period, while the other boreholes display stable or somewhat varying concentrations within the analytical uncertainty.

The charge balance errors give an indication of the quality and uncertainty of the analyses of major components. The errors do not exceed ±5% in any case.

The chloride concentrations are plotted versus the corresponding electrical conductivities in Figure 6-2. The plot provides a rough check that the values are reasonable.

Sulphate analysed by IC is plotted versus sulphate recalculated from total sulphur analysed by ICP technique in Figure 6-3. As shown, within the analytical error all sulphur is present as sulphate with some reservation for the samples with the highest concentrations. The results from ICP measurements are considered more reliable, by experience, since the variation in a time series often is smaller.

6.2 Isotope analysis

The isotope determinations include the stable isotopes δD, $\delta^{18}O$ and $^{10}B/^{11}B$ as well as the radioactive isotope ^3H (Trituim). The isotope data are compiled in Appendix 2, Table A2-2.

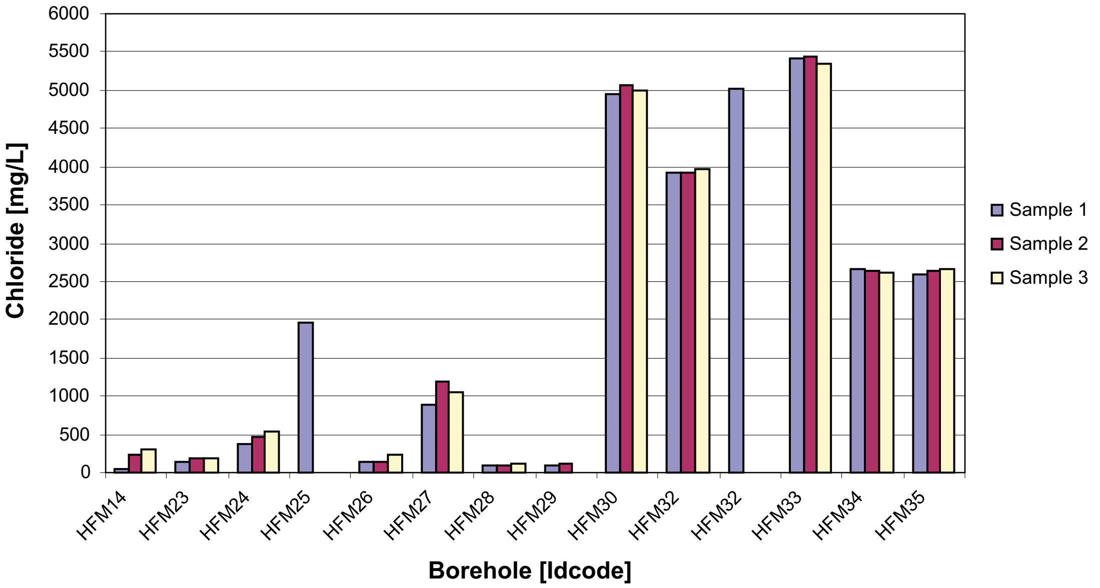

Figure 6-1. Chloride concentration series for boreholes HFM14, HFM23–30 and HFM32–35.

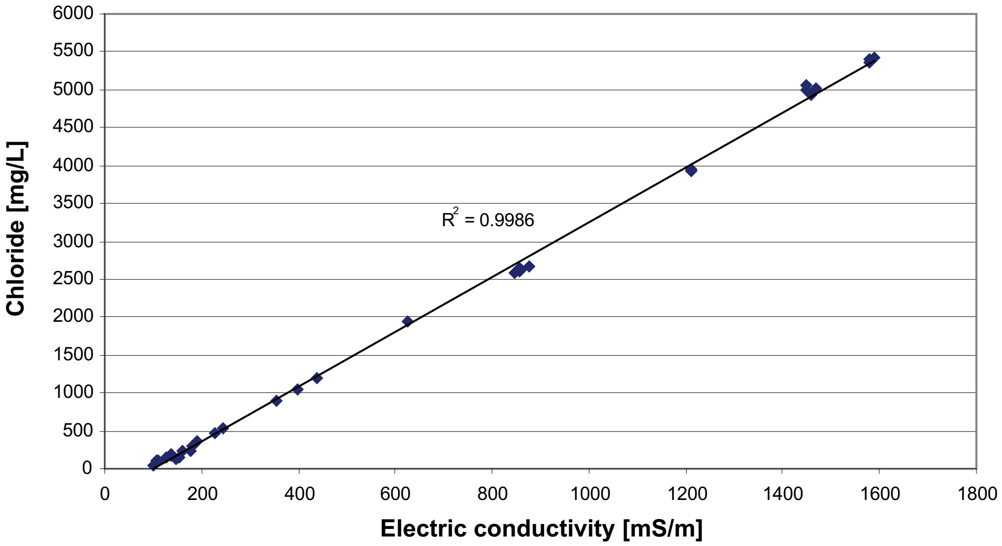

Figure 6-2. *Electrical conductivity versus chloride concentration.*

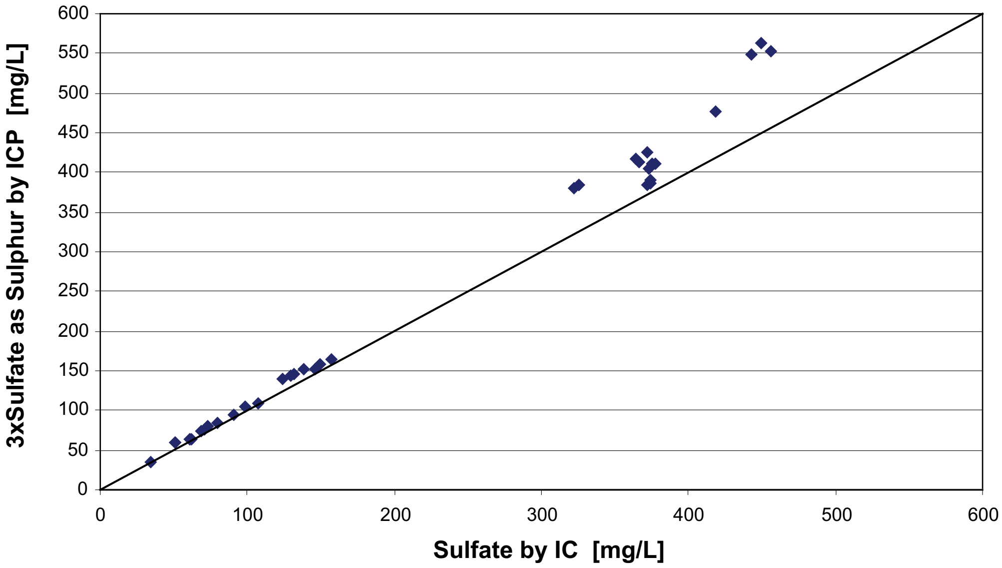

Figure 6-3. *Sulphate (SO_4 by IC) versus sulphate calculated from total sulphur ($3\times SO_4$–S by ICP).*

7 Summary and discussions

The sampling of groundwater from percussion drilled boreholes HFM14, HFM23–30 and HFM32–35 have been conducted in connection with hydraulic pumping tests performed in the boreholes from January to July, 2006. The experimental results can be summarized as follows:

- The chloride concentrations in boreholes HFM14, HFM23, HFM24, HFM26 and HFM35 show a slight increase during the pumping period. The other boreholes demontrate somewhat varying or stable chloride concentrations.
- It is recommended that the last sample in each series should be considered as the most representative for the groundwater in each borehole.
- The quality of the analytical data appears to be good. The relative charge balance error is below 5% for all collected samples and the checks by plotting show no obvious outliers.

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Appendix 1

Sampling and analytical methods

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

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within – or delivery time to lab.
Anions 1	HCO_3 pH(lab) cond (lab)	Plastic	250	Yes (not in the field)	No	Titration Pot. meas, Cond. meas	The same day – maximum 24 hours
Anions 2	Cl, SO_4, Br^-, F^-, I^-	Plastic	100	Yes (not in the field)	No	Titration (Cl^-) IC (Cl^-, SO_4, Br^-, F^-) ISE (F^-)	Not critical (month)
	Br, I	Plastic	100	Yes (not in the field)	No	ICP MS	Not critical (month)
Cations, Si and S according to SKB class 3	Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr	Plastic (at low conc. acid washed bottles)	100	Yes (not in the field)	Yes (not in the field, 1 mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Cations, Si and S according to SKB class 4 and 5	Na, K, Ca, Mg, S(tot), Si(tot), Fe, Mn, Li, Sr	Plastic (Acid washed)	100	Yes (immediately in the field)	Yes (1mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic (Acid washed)	500	Yes	Yes (5 mL HCl))	Spectrophotometry Ferrozine method	As soon as possible the same day
Hydrogen sulphide	HS-	Glass (Winkler)	About 120×2	No	Ev 1 mL 1 M NaOH+ 1 mL 1M ZnAc	Spectrophotometry	Immediately or if conserved, a few days
Environmental metals	Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn	Plastic (Acid washed)	100	Yes	Yes (1 mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Lantanoids, U, Th and so on.	Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th	Plastic (Acid washed)	100	Yes	Yes (1 mL HNO_3)	ICP-AES ICP-MS	Not critical (month)

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within – or delivery time to lab.
Dissolved organic Carbon, dissolved inorganic Carbon	DOC, DIC	Plastic	250 25	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time
Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within-or delivery time to lab.
Total organic Carbon	TOC	Plastic	250 25	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time
Environmental isotopes	^{2}H, ^{18}O	Plastic	100	No	– –	MS	Not critical (month)
Tritium	^{3}H (enhanced.)	Plastic (dry bottle)	500	No	–	LSC	
Chlorine-37	^{37}Cl	Plastic	100	No	–	ICP MS	Not critical (month)
Carbon isotopes	^{13}C, ^{14}C	Plastic (HDPE)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	^{34}S	Plastic	500–1,000	Yes	–	Combustion, MS	No limit
Strontium-isotopes	$^{87}Sr/^{86}Sr$	Plastic	100	Yes	–	TIMS	Days or Week
Uranium and Thorium isotopes	^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th,	Plastic	50 1,000	Nej	–	Chemical separat. Alfa/ gamma spectrometry	No limit
Boron isotopes	^{10}B	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP–MS	No limit
Radon and Radium isotopes	^{222}Rn, ^{226}Ra	Plastic	500–1,000	No	No	EDA, RD-200	Immediate transport
Dissolved gas (content and composition)	Ar, N_2, CO_2, O_2, CH_4, H_2, CO, C_2H_2, C_2H_4, C_2H_6, C_3H_8	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series	Polycarbonate filter	0.4, 0.2 and 0.05 µm	–	Ar atmosphere	ICP-AES ICP-MS	Immediate transport
Fractionation; Humic and fulvic acids, inorganic constituents	< 1,000 D > 1,000 D but < 5,000 D > 5,000 D	Fractions are collected in plastic bottles	250	–	N2 atmosphere	UV oxidation, IR (DOC)	Immediate transport
Archive samples with acid	–	Plast (washed in acid)	100×2 **	Yes	Yes (1 mL HNO_3)	–	Storage in freeze container

Component group	**Component/ element**	**Sample container (material)**	**Volume (mL)**	**Filtering**	**Preparation/ Conservation***	**Analysis method**	**Analysis within – or delivery time to lab.**
Archive samples without acid	–	Plastic	250×2 **	Yes	No	–	Storage in freeze container
Carbon isotopes in humic and fulvic acids	^{13}C, 1^4C (pmc)	DEAE cellulose (anion exchanger)	–	–	–	(A)MS	A few days
Nutrient salt + silicate	NO_2, NO_3, NO_2+NO_3, NH_4, PO_4, SiO_4	Sample tubes, plastic	25×2 250	Yes (in the field)	No, frozen immediately***	Spectrophotometry	Short transportation time
Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within-or delivery time to lab.
Total concentrations of Nitrogen and Phosphorous	N-tot, P-tot	Plastic	100	No	No, frozen immediately***	Spectrophotometry	Short transportation time
Particulate Carbon, Nitrogen and Phosphorous	POC, PON, POP	Plastic	1,000	Yes (within 4 h) prepared filters. Blank filters	Filtering, the filters are frozen immediately 2 filters/sample	Elementar-analysator (N, C) own method 990121 (P)	Short transportation time
Chlorophyll	Chlorophyll a, c and pheopigment	Plastic	1,000–2,000	Yes (within 4 h)	Filtering, the filters are frozen immediately	Spectrophotometry Fluorometry	Short transportation time
Oxygen	Dissolved O_2	Winkler, glass	2×ca 120	No	Mn (II) reagent Iodide reagent	Spectrophotometry SIS SS-EN 25813	Within 3 days
Archive samples for supplementary radio nuclides		Plastic	5,000	No	50 mL HNO_3	–	Storage in freeze container

* Suprapur acid is used for conservation of samples.

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

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

Abbreviations and definitions:

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

Table A1-2. Reporting limits and measurement uncertainties.

Component	Method	Reporting limits or range	Unit	Measurement uncertainty 2	”Total” uncertainty 3
HCO_3	Alkalinity titration	1	mg/L	4%	< 10%
Cl^- Cl^-	Mohr- titration IC	> 70 1–100	mg/L	5% 6%	< 10% 10%
SO_4	IC	1	mg/L	10%	15%
Br^- Br^-	IC ICP	0.2 0.001	mg/L	9% 15%	20%
F^- F^-	IC Potentiometric	0.1 –	mg/L	10% –	20%
I^-	ICP	0.001	mg/L	15%	20%
Na	ICP	0.1	mg/L	4%	10%
K	ICP	0.4	mg/L	6%	15%
Ca	ICP	0.1	mg/L	4%	10%
Mg	ICP	0.09	mg/L	4%	10%
S(tot)	ICP	0.160	mg/L	21%	15%
Si(tot)	ICP	0.03	mg/L	4%	15%
Sr	ICP	0.002	mg/L	4%	15%
Li	ICP	0.2[1] 2	mg/L	10%	20%
Fe	ICP	0.4[1] 4	mg/L	6%	10%
Mn	ICP	0.03[1] 0.1	µg/L	8%	10%
Fe(II), Fe(tot)	Spectrophotometry	0.02 (DL = 0.005 mg/L)	mg/L	15% (> 30 µg/L)	20%
HS^-	Spectrophotometry	SKB 0.03 (DL = 0.02)	mg/L	10%	30%
NO_2 as N	Spectrophotometry	0.1	µg/L	2%	20%
NO_3 as N	Spectrophotometry	0.2	µg/L	5%	20%
NO_2+NO_3 as N	Spectrophotometry	0.2	µg/L	0.2 (0.2–20 µg/L) 2% (> 20 µg/L)	20%
NH_4 as N	Spectrophotometry	0.8	µg/L	0.8 (0.8–20 µg/L) 5% (> 20 µg/L)	20%
		50 (SKB)		20%	
PO_4 as P	Spectrophotometry	0.7	µg/L	0.7 (0.7–20 µg/L) 3% (> 20 µg/L)	20%
SiO_4	Spectrophotometry	1	µg/L	3% (> 200 µg/L)	–
O_2	Jodometric titration	0.2–20	mg/L	5%	–
Chlorophyll a, c pheopigment[4]	See Table A1-2	0.5	µg/L	5%	–
PON[4]	See Table A1-2	0.5	µg/L	5%	–
POP[4]	See Table A1-2	0.1	µg/L	5%	–
POC[4]	See Table A1-2	1	µg/L	4%	–
Tot–N[4]	See Table A1-2	10	µg/L	4%	–
Tot–P[4]	See Table A1-2	0.5	µg/L	6%	–
Al, Zn	ICP	0.2	µg/L	12%	20%[5]
Ba, Cr, Mo, Pb	ICP	0.01	µg/L	7–10%	20%[5]
Cd, Hg	ICP	0.002	µg/L	9 resp 5%	20%[5]
Co, V	ICP	0.005	µg/L	8 resp 5%	20%[5]
Cu	ICP	0.1	µg/L	8%	20%[5]
Ni	ICP	0.05	µg/L	8%	20%[5]
P	ICP	1	µg/L	6%	10%
As	1CP	0.01	µg/L	20%	Correct order of size (low conc.)

Component	Method	Reporting limits or range	Unit	Measurement uncertainty 2	”Total” uncertainty 3
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb	ICP	0.0051 0.05	µg/L	10%	Correct order of size (low conc.)
Sc, In, Th	ICP	0.05^1 0.5	µg/L	10%	Correct order of size (low conc.)
Rb, Zr, Sb, Cs, Tl	ICP	0.025^1 0.25	µg/L	10%	Correct order of size (low conc.)
Y, Hf	ICP	0.005^1 0.05	µg/L	10%	Correct order of size (low conc.)
U	ICP	0.001^1 -	µg/L	12%	Correct order of size (low conc.)
DOC	See Table A1-1	0.5	mg/L	8%	30%
TOC	See Table A1-1	0.1	mg/L	10%	30%
δ^2H	MS	2	‰ SMOW^5	1‰	–
δ^{18}O	MS	0.1	‰ SMOW^5	0.2‰	–
^{3}H	LSC	0.8 eller 0.1	TU^6	0.8 eller 0.1	Correct order of size
^{37}Cl	ICP MS	0.2‰° (20 mg/L)	‰ SMOC^7	–	–
δ^{13}C	A (MS)	–	‰ PDB^8	–	–
^{14}C pmc	A (MS)	–	PMC^9	–	–
δ^{34} S	ICP MS	0.2‰	‰ CDT^{10}	0.3‰	–
^{87}Sr/^{86}Sr	TIMS	–	No unit (ratio)^{11}	–	–
^{10}B/^{11}B	ICP MS	–	No unit (ratio)^{11}	–	–
^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th	Alfa spectr.	0.0005	Bq/L13	5%	–
^{222}Rn, ^{226}Rn	LSC	0.03	Bq/L	5%	–

1. Reporting limits at salinity ≤ 0.4% (520 mS/m) and ≤ 3.5% (3,810 mS/m) respectively.
2. Measurement uncertainty reported by consulted laboratory, generally 95% confidence interval.
3. Estimated total uncertainty by experience (includes effects of sampling and sample handling).
4. Determined only in surface waters and near surface groundwater.
5. Per mille deviation[13] from SMOW (Standard Mean Oceanic Water).
6. TU = Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of 10^{-18} (1 Bq/L Tritium = 8.45 TU).
7. Per mille deviation[13] from SMOC (Standard Mean Oceanic Chloride).
8. Per mille deviation[13] from PDB (the standard PeeDee Belemnite).
9. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age: $pmC = 100\times e^{((1,950-y-1.03t)/8,274)}$ where y = the year of the C-14 measurement and t = C-14 age.
10. Per mille deviation[13] from CDT (the standard Canyon Diablo Troilite).
11. Isotope ratio without unit.
12. The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232:
    1 ppm U = 12.4 Bq/kg^{238}U
    1 ppm Th = 3.93 Bq/kg^{232}Th.
13. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as: $\delta^yI = 1,000\times(K_{sample}-K_{standard})/K_{standard}$, where K = the isotope ratio and ^yI = ^{2}H, ^{18}O, ^{37}Cl, ^{13}C or ^{34}S etc.

Appendix 2

Compilation of water analysis data

Table A2-1. Water composition.

Idcode	Secup m	Seclow m	Sample no.	Sampling date and time	RCB %	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	Li mg/L	Sr mg/L	pH	TOC mg/L	ElCond mS/m
HFM14	0	150.5	12220	2006-04-04 09:42	–0.39	28.8	5.93	167	11.0	520	50.6	34.5	11.9	0.21	0.65	7.62	0.006	0.240	6.67	19	99.4
HFM14	0	150.5	12219	2006-04-04 16:00	1.24	156	8.79	166	16.3	489	234	68.3	25.0	0.84	0.93	8.93	0.009	0.424	6.90	16	160
HFM14	0	150.5	12221	2006-04-04 20:00	0.04	196	9.06	158	16.9	469	302	79.8	28.1	1.04	1.03	8.58	0.010	0.454	6.94	15	181
HFM23	0	211.5	12054	2006-03-20 10:10	–1.31	165	7.48	76.7	16.9	435	147	71.3	25.4	0.46	1.21	8.66	0.014	0.520	7.38	13	126
HFM23	0	211.5	12053	2006-03-20 14:00	–1.57	180	7.40	77.9	17.0	425	179	73.5	26.5	0.57	1.23	8.60	0.015	0.547	7.34	12	136
HFM23	0	211.5	12050	2006-03-20 19:00	–0.35	189	7.75	81.3	17.5	427	188	73.4	26.5	0.62	1.22	8.77	0.015	0.579	7.33	13	137
HFM24	0	151.4	12065	2006-02-07 08:45	–1.87	289	11.9	76.1	17.6	396	365	91.2	31.5	1.28	1.51	6.51	0.171	0.537	7.65	10	191
HFM24	0	151.4	12064	2006-02-07 12:25	–1.41	329	13.0	92.5	21.6	380	467	99.0	34.9	1.68	1.42	6.84	0.173	0.643	7.64	10	228
HFM24	0	151.4	12059	2006-02-07 18:45	–2.28	349	13.5	100	23.6	379	531	107	36.1	1.93	1.48	6.82	0.177	0.696	7.58	10	243
HFM25	0	187.5	12058	2006-03-01 10:35	–1.05	781	13.4	402	68.0	198	1,950	124	46.8	7.16	1.66	5.71	0.040	4.57	7.29	6.2	624
HFM26	0	202.7	12056	2006-02-09 11:17	–1.44	295	7.64	30.5	5.8	518	129	146	50.8	0.39	3.13	6.95	0.011	0.230	7.92	11	148
HFM26	0	202.7	12055	2006-02-09 15:20	–0.38	307	7.77	32.4	6.1	513	139	149	52.7	0.40	3.19	7.10	0.011	0.247	7.89	10	153
HFM26	0	202.7	12049	2006-02-09 20:22	–0.32	332	8.10	54.1	9.2	501	228	157	54.8	0.69	3.05	7.16	0.012	0.424	7.89	10	178
HFM27	0	127.5	12061	2006-03-06 11:05	–2.76	455	19.1	172	42.4	357	890	138	50.4	3.00	1.44	6.46	0.021	1.17	7.61	7.2	355
HFM27	0	127.5	12060	2006-03-06 15:13	–0.21	598	17.5	248	37.9	330	1,190	132	48.9	5.05	1.59	6.48	0.021	2.03	7.63	6.4	438
HFM27	0	127.5	12057	2006-03-06 20:15	–0.45	551	17.5	208	36.5	350	1,040	130	47.7	4.35	1.53	6.54	0.019	1.60	7.65	7.2	399
HFM28	0	151.2	12052	2006-03-15 09:17	–1.46	162	5.26	54	9.4	427	91.4	61.3	21.2	0.39	1.37	7.71	0.013	0.442	7.57	11	107
HFM28	0	151.2	12037	2006-03-15 13:16	–1.53	165	5.74	54	10.0	429	98.6	61.0	20.9	0.36	1.37	7.97	0.013	0.45	7.59	12	108
HFM28	0	151.2	12051	2006-03-15 17:50	–2.11	163	5.80	55.6	10.3	425	106	62.1	20.9	0.45	1.39	7.97	0.013	0.46	7.54	12	109
HFM29	0	199.7	12255	2006-05-15 15:10	0.52	205	7.76	37.2	7.7	443	102	50.5	19.8	0.37	2.09	7.65	0.015	0.282	7.95	8.5	108
HFM29	0	199.7	12257	2006-05-15 17:20	0.41	207	7.83	37.5	7.7	442	107	51.2	19.9	0.30	2.14	7.59	0.015	0.283	8.14	10	110

Idcode	Secup m	Seclow m	Sample no.	Sampling date and time	RCB %	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	Li mg/L	Sr mg/L	pH	TOC mg/L	ElCond mS/m
HFM30	0	200.75	12256	2006-05-17 10:05	2.28	1,140	6.63	1,970	90.1	90.2	4,940	322	127	19.8	1.17	7.26	0.045	24.1	7.32	1.9	1,460
HFM30	0	200.75	12258	2006-05-17 14:04	1.18	1,140	6.43	1,980	90.6	96.0	5,070	326	128	20.6	1.09	7.54	0.048	24.1	7.34	1.8	1,450
HFM30	0	200.75	12259	2006-05-17 20:04	1.75	1,130	6.30	1,980	89.8	97.7	4,990	326	128	20.5	1.11	7.68	0.051	23.9	7.31	2.0	1,450
HFM32	0	202.65	12035	2006-01-17 09:40	–1.58	1,730	58.0	557	173	183	3,930	377	137	15.7	1.75	6.95	0.054	3.55	7.12	3.0	1,210
HFM32	0	202.65	12034	2006-01-17 14:02	–1.48	1,640	54.1	625	180	182	3,920	375	137	15.5	1.41	7.16	0.048	3.24	7.16	3.0	1,210
HFM32	0	202.65	12036	2006-01-17 18:00	–3.14	1,680	55.8	546	170	180	3,960	373	135	14.9	1.57	7.21	0.052	3.54	7.15	2.9	1,210
HFM32	50	202.65	12066	2006-01-18 15:20	–2.89	1,840	30.1	954	196	107	5,010	419	159	19.1	1.78	7.02	0.058	8.21	7.50	1.8	1,470
HFM33	0	140.2	12245	2006-05-09 07:52	–1.73	2,060	31.4	1,000	248	118	5,410	449	188	19.0	1.20	7.53	0.061	9.17	7.23	1.4	1,580
HFM33	0	140.2	12246	2006-05-09 11:55	–1.17	2,110	32.7	1,000	248	123	5,430	456	184	19.3	1.21	7.66	0.062	9.06	7.30	1.4	1,590
HFM33	0	140.2	12247	2006-05-09 15:55	–0.36	2,090	33.4	1,020	251	125	5,350	443	183	18.8	1.22	7.68	0.062	8.88	7.32	1.3	1,580
HFM34	0	200.75	12289	2006-06-08 08:44	–1.22	1,450	59.3	89.4	170	98.7	2,650	366	138	8.50	0.41	1.22	0.029	1.14	7.82	3.0	855
HFM34	0	200.75	12290	2006-06-08 11:55	–1.03	1,450	58.7	89.8	170	98.8	2,630	372	142	8.50	0.41	1.24	0.03	1.12	7.75	3.1	859
HFM34	0	200.75	12291	2006-06-08 17:15	–0.38	1,460	60.0	87.4	170	99.2	2,610	364	139	8.55	0.40	1.22	0.029	1.13	7.75	3.0	857
HFM35	0	200.75	12327	2006-07-04 10:40	–1.14	1,420	45.8	137	147	157	2,590	372	128	9.20	0.88	4.99	0.028	1.43	7.70	2.0	848
HFM35	0	200.75	12328	2006-07-04 14:57	–0.80	1,430	41.7	170	144	154	2,630	374	130	9.70	0.84	4.87	0.029	1.84	7.70	2.0	856
HFM35	0	200.75	12329	2006-07-04 20:01	–1.52	1,380	39.6	211	144	153	2,670	374	129	9.60	0.95	4.95	0.03	2.41	7.68	1.9	878

– = Not analysed.

A = Results will be reported later.

x = No result due to sampling problems.

< ”value” = below reporting limit.

RCB % = Rel. charge balance error %.

SICADA: water_composition.

Table A2-2. Isotopes I (H-, O- and B-isotopes).

Idcode	Secup m	Seclow m	Sample no	Sampling date	δ^2H dev SMOW	^3H TU	$\delta^{18}O$ dev SMOW	$^{10}B/^{11}B$ no unit
HFM14	0	150.5	12221	2006-04-04	–82.3	8.1	–11.5	0.2388
HFM23	0	211.5	12050	2006-03-20	–79.9	9.1	–11.0	0.2397
HFM24	0	151.4	12059	2006-02-07	–80.1	5.9	–10.5	0.2373
HFM25	0	187.5	12058	2006-03-01	–88.3	2.5	–11.9	0.2389
HFM26	0	202.7	12049	2006-02-09	–80.2	1.9	–10.5	0.2372
HFM27	0	127.5	12057	2006-03-06	–80.8	7.6	–10.9	0.2389
HFM28	0	151.2	12051	2006-03-15	–79.6	9.9	–10.9	0.2402
HFM29	0	199.7	12257	2006-05-15	–85.2	6.5	–11.5	0.2403
HFM30	0	200.75	12259	2006-05-17	–94.0	1.0	–12.4	0.2406
HFM32	0	202.65	12036	2006-01-17	–68.4	< 0.8	–9.1	0.2377
HFM32	50	202.65	12066	2006-01-18	–71.8	1.7	–9.8	0.2388
HFM33	0	140.2	12247	2006-05-09	–67.7	1.2	–8.7	0.2396
HFM34	0	200.75	12291	2006-06-08	–64.3	13.5	–8.3	0.2391
HFM35	0	200.75	12329	2006-07-04	–66.3	10.0	–8.6	0.2387

– = Not analysed.

A = results will be reported later.

xx = No result due to analytical problems.

< ”value” = below reporting limit
SICADA: isotopes_1.