

P-05-187

Forsmark site investigation

Hydrochemical logging in KFM07A

Cecilia Berg, Jacob Levén, Ann-Chatrin Nilsson
Geosigma AB

June 2005

Svensk Kärnbränslehantering AB

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



ISSN 1651-4416

SKB P-05-187

Forsmark site investigation

Hydrochemical logging in KFM07A

Cecilia Berg, Jacob Levén, Ann-Chatrin Nilsson
Geosigma AB

June 2005

Keywords: Core drilled borehole, Groundwater, Water sampling, Tube sampling, Up-coning effect, Chemical analyses, AP PF 400-05-033.

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.

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

Abstract

Hydrochemical logging or so called tube sampling has been performed in the core drilled borehole KFM07A. The method offers a fast and simple sampling technique for obtaining information about the chemical composition of the water column along an open borehole. The equipment consists of an approximately 1,000 m long polyamide tube divided into units of 50 m.

Generally, the water content in each tube unit constituted one sample and every other sample was analysed. Two samples (from sections 100–200 m and 450–550 m) were, however, concatenated from two tube units in order to allow analyses of all SKB class 3 isotope options. The isotope options were included for samples below 350 m borehole length. Above that length, the samples showed too high flushing water contents ($> 20\%$) to be of interest. The relative charge balance error did not exceed the acceptable level of $\pm 5\%$ in any of the eight samples analysed.

The analytical results show quite low flushing water contents ($< 3\%$) below 450 m borehole length and chloride concentrations as high as between 13,600–14,300 mg/L. However, due to heavy pumping during and after drilling, the borehole was filled to the ground surface with saline water which may originate from the fracture at 970 m borehole length or from even larger depths.

Sammanfattning

Hydrokemisk loggning, eller så kallad slangprovtagning, har utförts i det kärnborrade borrhålet KFM07A. Metoden är snabb och enkel att använda för att erhålla information om den kemiska sammansättningen hos grundvattnet längs ett öppet borrhål. Utrustningen består av en cirka 1 000 m lång polyamidslang uppdelad i enheter om vardera 50 m.

Normalt utgjorde innehållet i en slangenhet ett prov och vartannat prov analyserades. Två av proven (från sektionerna 100–200 m samt 450–550 m) bestod dock av vatten från två slangenheter för att ge tillräcklig vattenvolym för analys av samtliga isotoptillval enligt SKB kemiklass 3. Isotoptillval inkluderades för prover tagna under 350 m borrhålslängd. Ovanför denna längd visade proven för höga spolvattenhalter (> 20 %) för att vara av intresse. Det relativa felet i jonbalansen överskred inte gränsen för vad som är acceptabel nivå ($\pm 5\%$) i något av de åtta analyserade proven.

Resultaten från analyserna visar på rätt låga spolvattenhalter (< 3 %) under 450 m borrhålslängd och så höga kloridkoncentrationer som mellan 13 600–14 300 mg/L. På grund av kraftig pumpning under och efter borringen, fylldes emellertid borrhålet hela vägen upp till ytan med salt vatten som kan härröra från en spricka vid 970 m borrhålslängd eller från ännu större djup.

Contents

1	Introduction	7
2	Objective and scope	9
3	Background	11
4	Sampling equipment	13
5	Performance	15
5.1	Hydrochemical logging	15
5.2	Sample treatment and chemical analysis	15
5.3	Data handling	16
5.4	Nonconformities	18
6	Results	19
7	Summary and discussion	21
8	References	23
	Appendix 1 Design of cored borehole KFM07A	25
	Appendix 2 Picture from BIPS logging in KFM07A	27
	Appendix 3 Sampling and analysis methods	29
	Appendix 4 Water composition, compilation of basic water analysis data	33
	Appendix 5 Isotopes, compilation of H-, O-, B-, S-, Cl-, Sr- and C-isotopes	35

1 Introduction

This document reports performance and results of the activity *Hydrochemical logging* in KFM07A within the site investigation programme at Forsmark /1/. The work was conducted according to the activity plan AP PF 400-05-033 (SKB internal controlling document). The fieldwork was carried out in March 2005. The controlling documents for the activity are listed in Table 1-1. Both activity plan and method description are SKB's internal controlling documents.

Borehole KFM07A is the seventh deep telescopic borehole drilled at the site investigation in Forsmark /2/. The location of KFM07A and the other current deep telescopic boreholes within the investigation area are shown in Figure 1-1. Figure 1-2 shows a zooming in towards drill site DS7 with KFM07A, and nearby situated percussion drilled boreholes in soil and rock. The borehole KFM07A is inclined 60° from the horizontal plane in the direction towards north-west. The borehole section 0–100.40 m is percussion drilled and has a stainless steel casing with the internal diameter of 200 mm, section 100.40–101.70 is core drilled with the diameter 86.0 mm and cased, whereas section 101.70–1,001.55 m is core drilled with a diameter of 77.3 mm. The design of the borehole KFM07A 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 610.003 (Method description for percussion drilling). An SKB chemical type of borehole requires cleaning procedures of all equipment to be used in the borehole, during and after drilling, according to level 2 in the cleaning instructions in MD 600.004 (Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning).

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

Activity plan	Number	Version
Hydrokemisk loggning i KFM07A	AP PF 400-05-033	1.0
Method descriptions	Number	Version
Metodbeskrivning för hydrokemisk loggning	SKB MD 422.001	1.0
Instruktion för rengöring av borrhålsutrustning och viss markbaserad utrustning	SKB MD 600.004	1.0

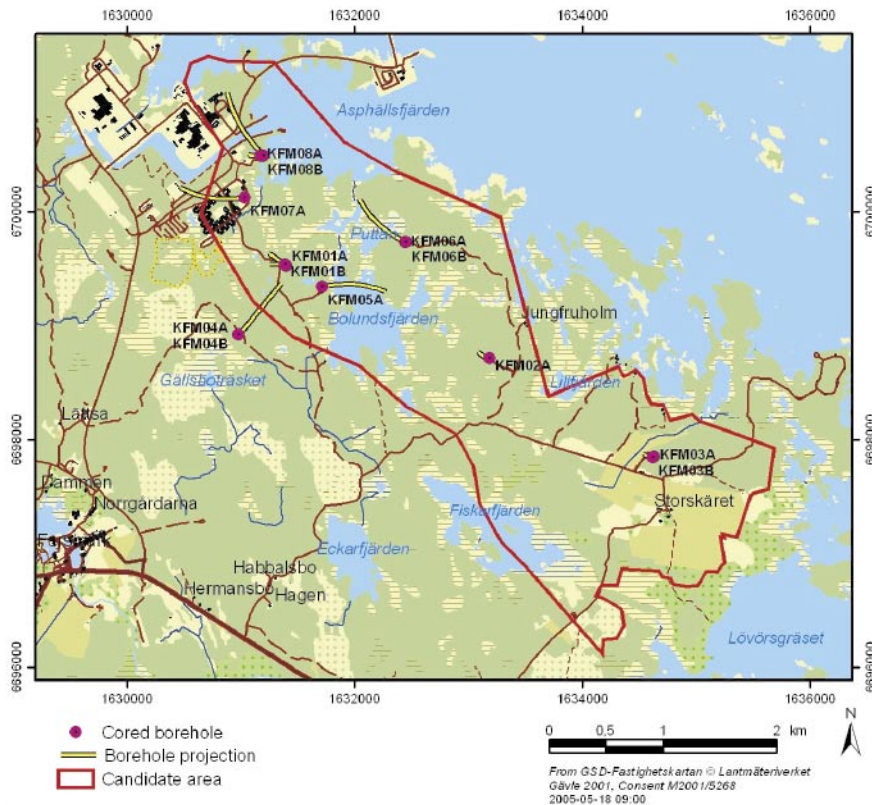


Figure 1-1. The investigation area at Forsmark (approximately the area inside the black square) including the candidate area selected for more detailed investigations. The deep and semi-deep (c 100–450 m) cored boreholes, KFM01A to KFM08B, are marked with pink circles.

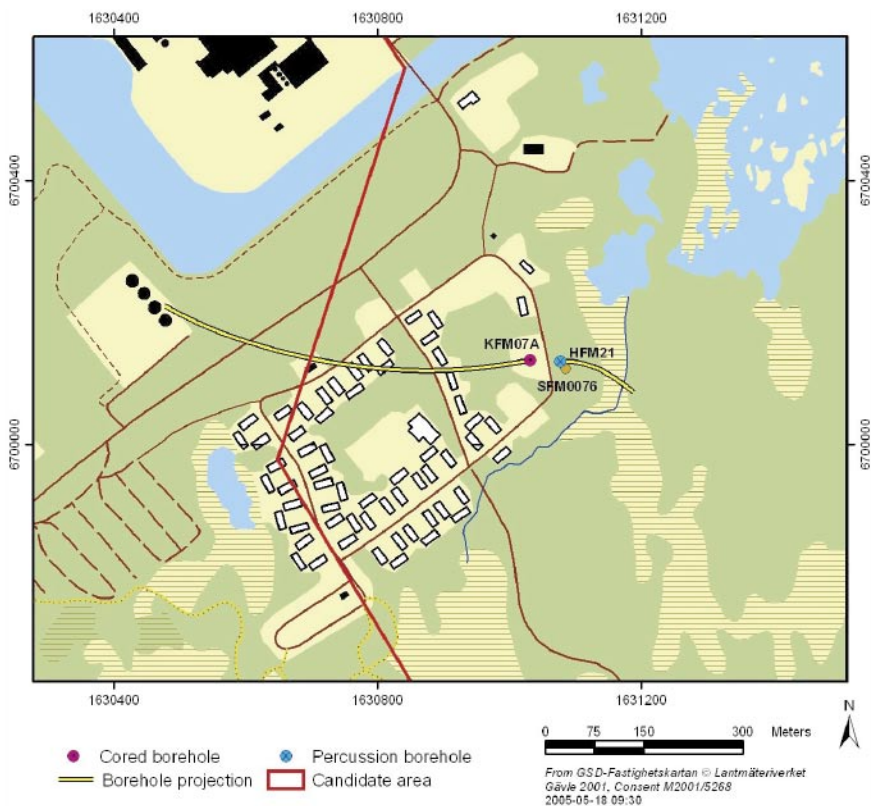


Figure 1-2. Location and projection on the horizontal plane of the cored borehole KFM07A, the percussion borehole HFM21 and the shallow monitoring well in soil SFM0076 at drill site DS7.

2 Objective and scope

Hydrochemical logging was performed in order to obtain an overview of the initial chemical composition of the water column along the open borehole KFM07A. The technique used for sampling is fast and simple even at great depths.

The analysis program was carried out according to SKB chemistry class 3 including isotope options. However, if the content of flushing water remaining from core drilling exceeded 25% in a sample the isotope determinations were omitted.

3 Background

Events and activities in the borehole prior to the hydrochemical logging are listed in Table 3-1.

Table 3-1. Activities performed in KFM07A prior to the hydrochemical logging.

Activities performed	Date of completion	Length or section (m)	Comment
Percussion drilling	2004-06-16	0–100.40	
Core drilling	2004-12-09	100.40–1,001.55	HFM21 provided the source of flushing water for drilling of the cored part of KFM07A. HFM21 is an SKB chemical type of borehole /2, 3, 4/.
Flushing water treatment	–	–	Automatic dosage of Uranine was applied during drilling of KFM07A. In this way no in-line storage tank was needed after the UV-system /2/.
Microbe control was not performed		–	–
WL water sampling SKB class 3	2004-10-28	100.4–305.84	Sample no. 8712.
BIPS-logging	2005-01-11	101–950	/5/
Radar logging	2005-01-14	100– approx 990	The equipment was lowered to different depths at different occasions.
Differential flow logging	2005-01-29	100– approx 990	The equipment was lowered to different depths and did not reach the bottom at all logging occasions. The reason was problems with out-falls in the borehole /6/.
BIPS-logging	2005-02-09	550–993	/5/
Geophysical logging	2005-02-09	102– approx	/7/
Injection tests (PSS3)	2005-03-01	104–1,001.55	Due to logistic advantages, injection tests were performed before the hydrochemical logging /8/.
Hydrochemical logging	2005-03-09	0–850	Presented in this report.

4 Sampling equipment

The equipment used for *hydrochemical logging* consists of an approximately 1,000 m long polyamide tube, divided into units of 50 m (SKB MD 422.001).

A schematic illustration of the equipment is presented in Figure 4-1. The length of each tube unit is approximately 50 m. The units are connected with metal couplings, and manual shut off valves are mounted at both ends of each unit. The external and internal diameters of the tube units are 10 and 8 mm respectively. The water content in each tube unit constitutes one sample and the volume of each sample will amount to at least two litres. A check valve and a weight are mounted at the bottom of the tube array to prevent water outflow and to keep the array stretched in the borehole.

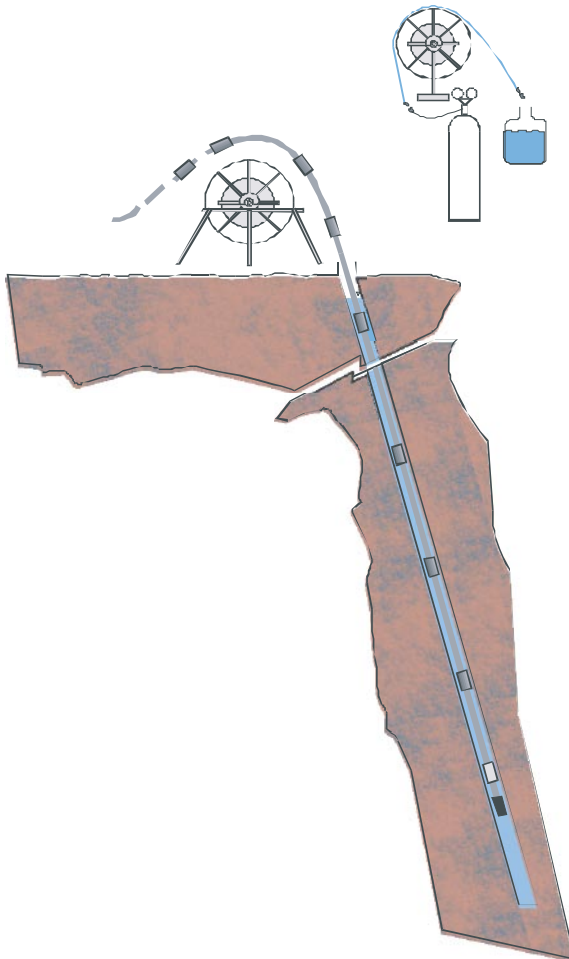


Figure 4-1. Equipment for hydrochemical logging in boreholes. At the lower end of the tube array there is a non-return valve and a weight connected. Each tube unit is 50 m long.

5 Performance

5.1 Hydrochemical logging

Sampling of the telescopic borehole KFM07A was performed on the 9: th of March 2005 according to the activity plan AP PF 400-05-033 and following the method description SKB MD 422.001.

The hydrochemical logging was performed to a length of 850 m down the borehole. The reason why the tube array was not lowered all the way down to the bottom of the borehole was blocking by out-falls at about 855 m borehole length, see BIPS-picture in Appendix 2. The lowering of the tubes started at 09:13 and the retrieval of the tube units started at 12:35. The tube units were emptied using pressurized nitrogen gas and the water was portioned into plastic bottles to be analysed at different laboratories. In most cases one tube unit constitutes one sample. However, samples SKB nos 8812 and 8818 consist of two concatenated tube units in order to allow analyses of all SKB class 3 isotope options. The groundwater level in the borehole was 9.47 m from the top of the casing just before sampling which resulted in that the upper tube unit that was not completely filled.

5.2 Sample treatment and chemical analysis

A table presenting sample treatment and analysis routines is given in Appendix 3. The routines are applicable independent of sampling object or sampling method. An overview showing the filled sample portions at the logging occasion is given in Table 5-1. The samples SKB nos 8810, 8812 and 8814 intended for isotope analyses were not sent to the laboratories for isotope determination due to their high amount of remaining flushing water from drilling (more than 20%). The data from the hydrochemical logging are stored in the database SICADA, where they are traceable by the activity plan number. The SKB sample numbers are 8810–8824.

Table 5-1. Overview of samples collected at the hydrochemical logging in KFM07A. Filled cells represent collected samples. Dark grey cells represent collected archive samples.

Sample information			Collected sample portions										
Tube unit	Length (m)	SKB no	Cond, pH, alk.	Major constit.	Br-/I- Anions	Uranine	³ H	$\delta^2\text{H} / \delta^{18}\text{O}$	$\delta^{37}\text{Cl}$	⁸⁷ Sr	C-isotopes	$\delta^{34}\text{S}$	Left over
1	0-50	8810					x	x	x	x	x		
2	100	8811											
3&4	200	8812					x	x	x	x	x	x	
5	250	8813											
6	300	8814											
7	350	8815											
8	400	8816											
9	450	8817											
10&11	550	8818											
12	600	8819											
13	650	8820											
14	700	8821											
15	750	8822											
16	800	8823											
17	850	8824											

x = samples were collected but not analysed due to high flushing water content.

5.3 Data handling

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

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

All analytical results were 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 $\pm 5\%$ 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 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.

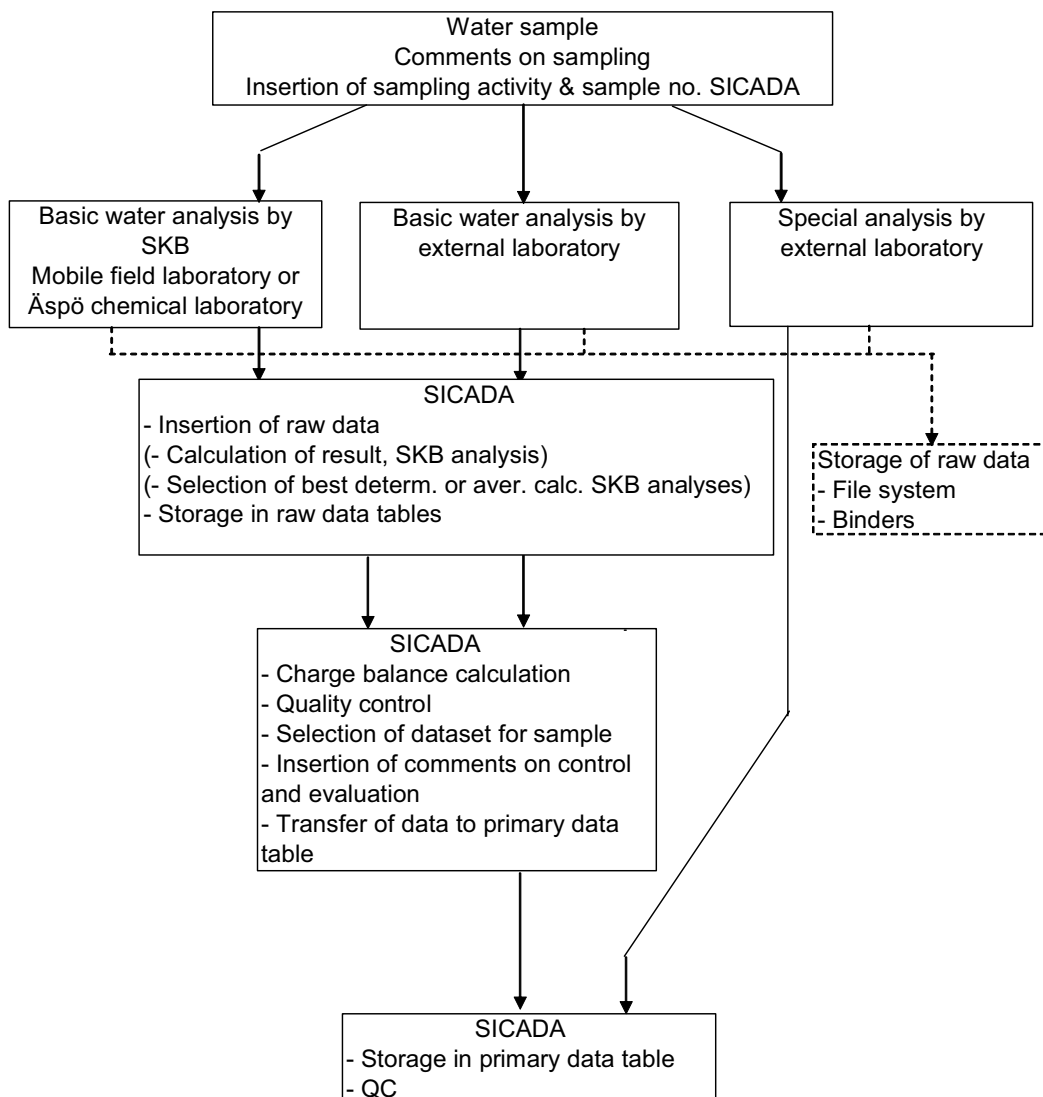


Figure 5-1. Overview of data management for hydrogeochemical data.

5.4 Nonconformities

The hydrochemical logging of KFM07A was on the whole performed according to activity plan and method description. However, due to out-fall blocking the borehole, the logging could only be performed to 850 m borehole length and not to the bottom of the borehole.

6 Results

The results from the chemical analyses are presented in Appendices 4 and 5. The flushing water content and the electric conductivity along the borehole are presented in Figures 6-1 and 6-2. The results are plotted for the mid-length of each tube unit. Since the flushing water content exceeds 20% in the upper part of the borehole (< 350 m), no isotope results are available from this part.

The charge balance errors give an indication of the quality and uncertainty of the analyses of major constituents. The relative charge balance errors calculated for the sets of data given in Appendix 4 do not exceed 5% in any of the cases.

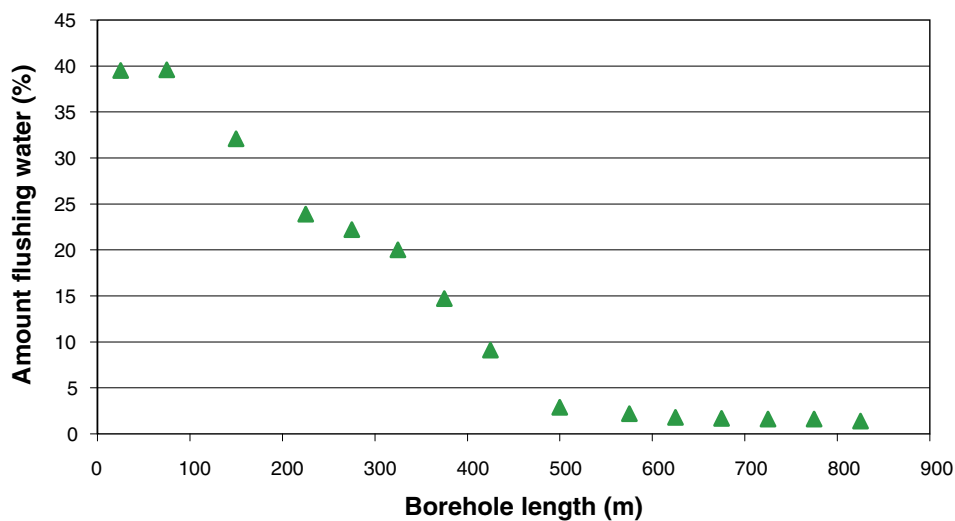


Figure 6-1. Content of remaining flushing water versus borehole length.

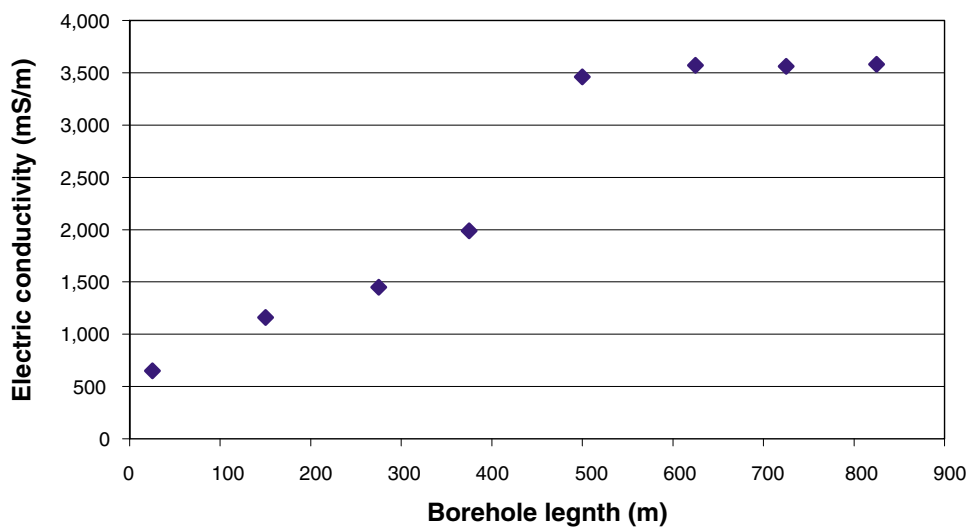


Figure 6-2. Electric conductivity versus borehole length.

7 Summary and discussion

The hydrochemical logging in borehole KFM07A revealed the chemical conditions of the water column along the borehole. The most striking observation is the up-coning of saline water due to heavy pumping during and after drilling of the borehole. The results of the analyses demonstrate low flushing water content ($< 3\%$) and an interestingly high salinity in the part of the borehole below 450 m borehole length. The depth from which this saline water originates is, however, somewhat uncertain. Isotope determinations were included for the samples below 350 m.

Figure 7-1, shows the position of the saline front at three occasions during unpumped as well as pumped conditions in connection with the difference flow logging campaign and at the hydrochemical logging.

Rinse pumping of KFM07A caused an up-coning of highly saline water from great depth in the borehole. This was first observed during the difference flow logging campaign c 2 weeks after stop of rinse pumping. The borehole has a steeply dipping, highly conductive fracture at c 970 m borehole length ($T \sim 6E-7 \text{ m}^2/\text{s}$), from which the saline water is assumed to originate. Apart from the fracture at c 970 m, no significant water-yielding fractures are found below c 250 m in the borehole.

During the 13 days of rinse pumping, a drawdown of c 4 m was obtained. Given the drawdown and the transmissivity of the fracture, a rough fracture-specific flow rate can be estimated at 0.14 L/min, due to rinse-pumping. The total volume of saline water withdrawn from the fracture at c 970 m into the borehole would then be c 2.7 m^3 , which correspond to the borehole volume of c 580 m. (diameter 77 mm). Together this would raise the saline water front up to c 390 m. However, this is a very rough estimation and the correct saline water volume might as well be the double.

The first difference flow logging measurements were carried out c 2 weeks after stop of rinse pumping. This would permit the saline water to subside compared to just after stop of pumping. The “falling velocity” of the saline water can be estimated by comparing the saline profiles from the difference flow logging with the hydrochemical logging, given the time between the measurements. The falling velocity can be estimated at c 4 m/day. Allowing 14 days of “falling velocity”, the expected saline water level should be found at c 450 m at the time for the difference flow logging. The saline water was, however, first found at c 340 m, indicating a slight underestimation of the up-coning in the exercise above.

Forsmark, borehole KFM07A
Electric conductivity of borehole water

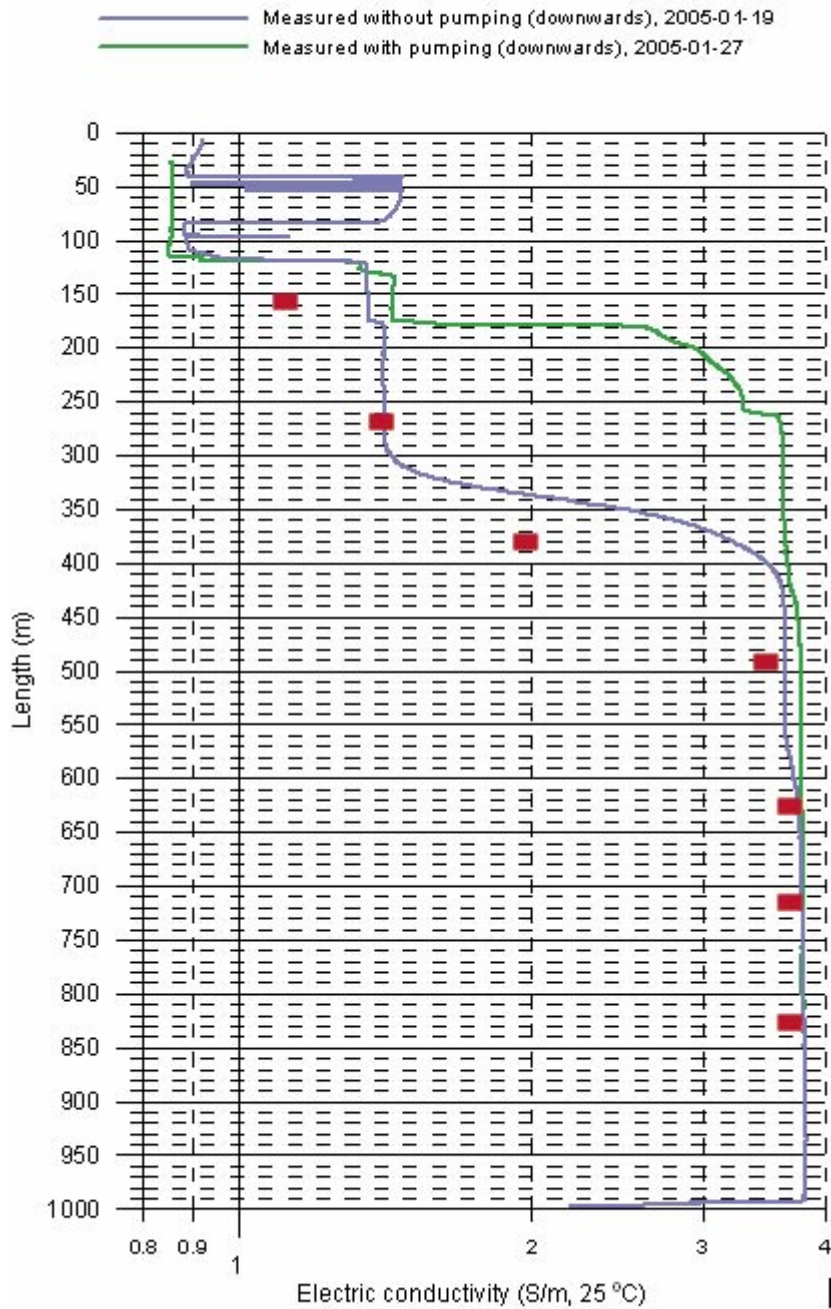


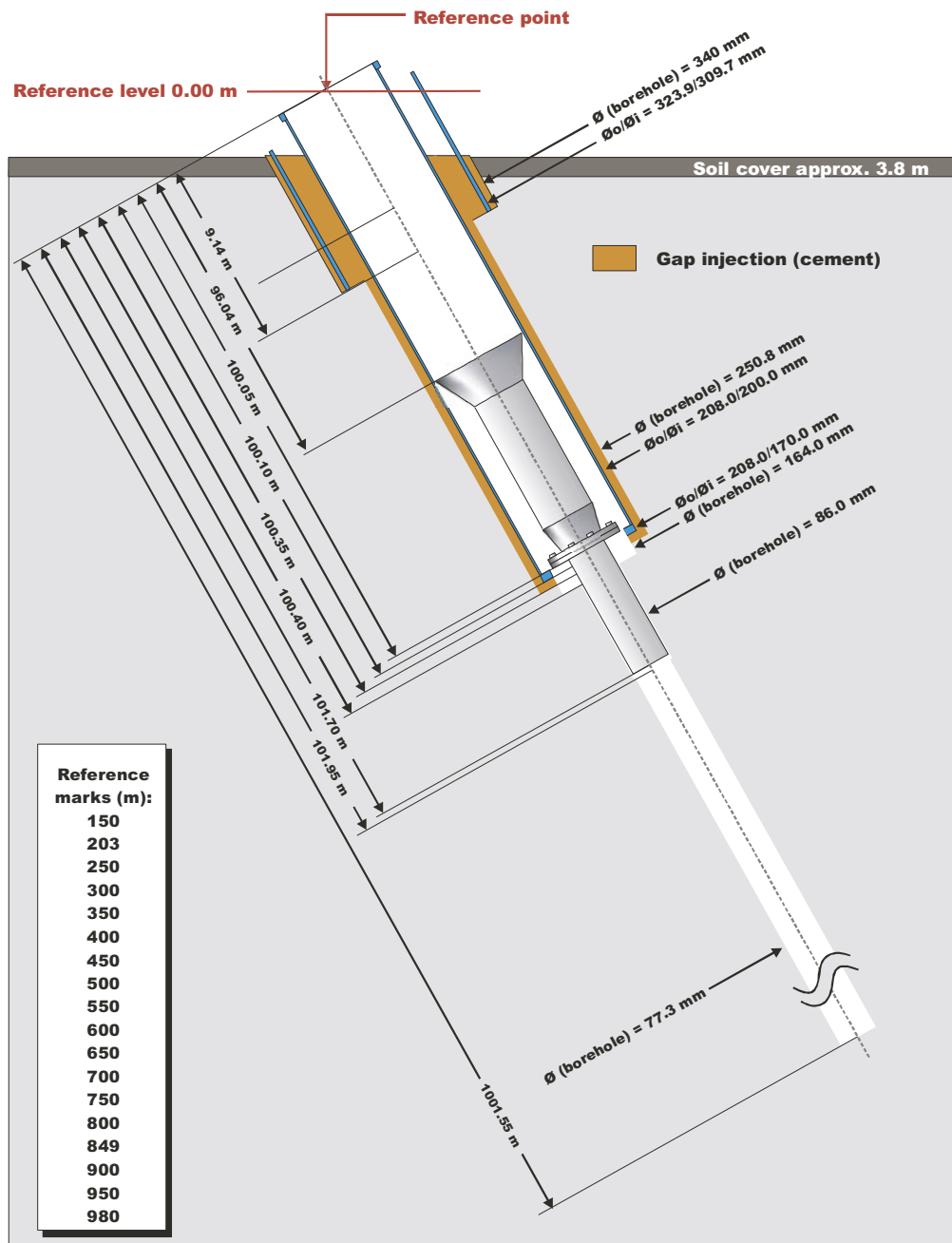
Figure 7-1. Electric conductivity in the groundwater along the borehole KFM07A at three dates; 2005-01-19 (blue), 2005-01-27 (green) and 2005-03-09 (red dots). The two first dates refer to the difference flow logging campaign and the last date to the hydrochemical logging.

8 References

- /1/ **SKB, 2001.** Site investigations. Investigation methods and general execution programme. SKB TR-01-29, Svensk Kärnbränslehantering AB.
- /2/ **Claesson L-Å, Nilsson G, 2005.** Forsmark site investigation. Drilling of the telescopic borehole KFM07A at drill site DS7. SKB P-05-142, Svensk Kärnbränslehantering AB.
- /3/ **Claesson L-Å, Nilsson G, 2005.** Forsmark site investigation. Drilling of two flushing water wells, HFM21 and HFM22, one groundwater monitoring well in solid bedrock, HFM20, and one groundwater monitoring well in soil, SFM0076. SKB P-04-245, Svensk Kärnbränslehantering AB.
- /4/ **Nilsson D, 2005.** Forsmark site investigation. Sampling and analyses of groundwater from percussion drilled boreholes. Results from the percussion drilled boreholes HFM20, HFM21 and HFM22. SKB P-05-48, Svensk Kärnbränslehantering AB.
- /5/ **Gustafsson J, Gustafsson C, 2005.** Forsmark site investigation. Ramac and BIPS logging in borehole KFM07A. SKB P-05-52, Svensk Kärnbränslehantering AB.
- /6/ **Rouhiainen P and Solonicki M, 2005.** Forsmark site investigation. Difference flow logging in borehole KFM07A. SKB P-05-63, Svensk Kärnbränslehantering AB.
- /7/ **Nielsen U T, Ringgaard J, Fris Dahl J, 2005.** Forsmark site investigation. Geophysical borehole loggings in the boreholes KFM07A, KFM08A and KFM08B. SKB P-05-159, Svensk Kärnbränslehantering AB.
- /8/ **Gokall-Norman K, Svensson T, Ludvigsson J-E, 2005.** Forsmark site investigation. Single-hole injection tests in borehole KFM07A. SKB P-05-133, Svensk Kärnbränslehantering AB.

Design of cored borehole KFM07A

Technical data Borehole KFM07A



Drilling reference point

Northing: 6700127.08 (m), RT90 2,5 gon V 0:-15
Easting: 1631031.57 (m), RT90 2,5 gon V 0:-15
Elevation: 3.32 (m), RHB 70

Orientation

Bearing (degrees): 261.47°
Inclination (degrees): -59.22°

Borehole

Length: 1001.55 m

Percussion drilling period

Drilling start date:
Drilling stop date:

Core drilling period

Drilling start date: 2004-10-18
Drilling stop date: 2004-12-09

Picture from BIPS logging in KFM07A

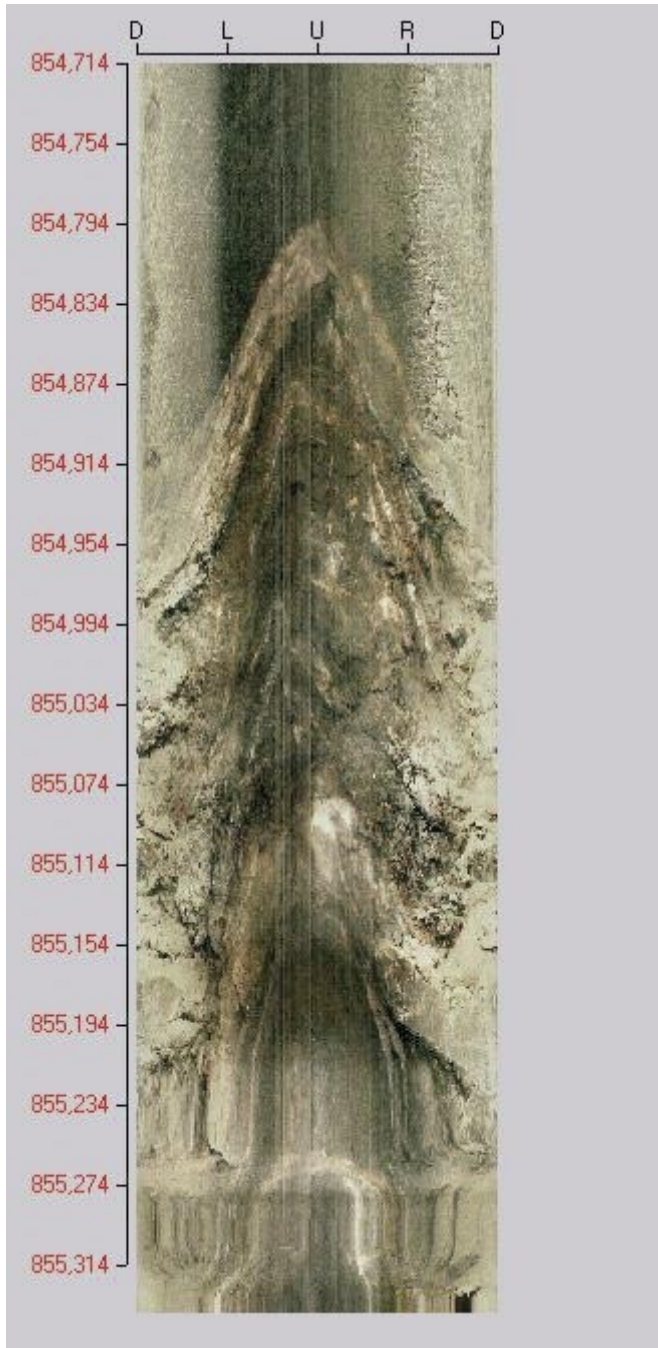


Figure A2-1. Borehole KFM07A: BIPS-image from 854.7–855.3 m.

Sampling and analysis methods
Table A3-1. 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.
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 120x2	No	Ev 1 mL 1 M NaOH+ 1 mL 1M ZnAc	Spectrophotometry	Immediately or if conserved, a few days
Nutrient salts	NO ₂ , NO ₃ +NO ₂ , NH ₄ , PO ₄	Plastic	250	No	No	Spectrophotometry	Maximum 24 hours
Environmental metals	Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Lantanoids, U, Th and so on:	Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th	Plastic	100	Yes	Yes (1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within – or delivery time to lab.
Dissolved organic Carbon, dissolved inorganic Carbon	DOC, DIC	Plastic	250 25	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analyser Shimadzu TOC5000	Short transportation time
Total organic Carbon	TOC	Plastic	250 25	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analyser Shimadzu TOC5000	Short transportation time
Environmental isotopes	^2H , ^3H	Plastic	100	No	–	MS	Not critical (month)
Tritium,	^3H (enhanced.)	Plastic (dry bottle) Plastic	500	No	–	LSC	Not critical (month)
Chlorine-37	^{37}Cl		100	No	–	ICP MS	
Carbon isotopes	^{13}C , pmC (^{14}C)	Glass (brown)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	^{34}S	Plastic	500 –1,000	Yes	–	Combustion, ICP MS	No limit
Strontium-isotopes	$^{87}\text{Sr}/^{86}\text{Sr}$	Plastic	100	Yes	–	TIMS	Days or Week
Uranium and Thorium isotopes	^{234}U , ^{235}U , ^{238}U , ^{232}Th , ^{230}Th ,	Plastic	50	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	500	No	No	EDA, RD-200	Immediate transport
Dissolved gas (content and composition)	Ar, N ₂ , CO ₂ , O ₂ , CH ₄ , H ₂ , CO, C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₈	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series and fractionation (see below)	Polycarbonate filter	0.45, 0.2 and 0.05 µm	–	N ₂ atmosphere	ICP-AES ICP-MS	Immediate transport
Humic and fulvic acids	Fractionation	Fractions are collected in plastic bottles	250	–	N ₂ atmosphere	UV oxidation, IR (DOC)	Immediate transport
Archive samples with acid	–	Plast (washed in acid)	100×2 **	Yes	Yes (1 mL HNO_3)	–	Storage in freeze container
Archive samples without acid	–	Plastic	250×2 **	Yes	No	–	Storage in freeze container
Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.
Carbon isotopes in humic and fulvic acids	^{13}C , pmC (^{14}C)	DEAE cellulose (anion exchanger)	–	–	–	(A)MS	A few days

* 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.

Abbreviations and definitions:

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

Table A3-2. 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 %
Cl ⁻	Mohr titration	5	70	mg/L	5 %	< 10 %
Cl ⁻	IC	0.2	0.5		6 %	10 %
SO ₄	IC	0.2	0.5	mg/L	6 %	15 %
Br ⁻	IC	0.2	0.7	mg/L	9 %	20 %
Br ⁻	ICP	–	0.001–0.010 ¹		15 %	
F ⁻	IC	0.2	0.6	mg/L	10 %	20 %
F ⁻	Potentiometri	–	–		–	–
I ⁻	ICP	–	0.001–0.010 ¹	mg/L	15 %	20 %
Na	ICP	–	0.1	mg/L	4 %	10 %
K	ICP	–	0.4	mg/L	6 %	15 %
Ca	ICP	–	0.1	mg/L	4 %	10 %
Mg	ICP	–	0.09	mg/L	4 %	10 %
S(tot)	ICP	–	0.160	mg/L	10 %	15 %
Si(tot)	ICP	–	0.03	mg/L	4 %	15 %
Sr	ICP	–	0.002	mg/L	4 %	15 %
Li	ICP	–	0.2–2 ¹	µg/L	10 %	20 %
DOC	See tab. 1	–	0.5	Mg/L	8 %	30 %
TOC	See tab. 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 kol	PmC ⁸	–	–
Component	Method	Detection limit	Reporting limit or range	Unit	Measurement uncertainties ²	“Total” uncertainties ³
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,	Alfa spectr.	–	0.05	Bq/L ¹³¹	0.05 Bq/L	Right order of magnitude
²³² Th, ²³⁰ Th						
²²² Rn, ²²⁶ Rn	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 deviation¹² 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 deviation¹² from SMOC (Standard Mean Oceanic Chloride).
- Per mill deviation¹² from PDB (the standard PeeDee Belemnite).
- The following relation is valid between pmC (percent modern carbon) and Carbon-14 age:

$$\text{pmC} = 100 \times e^{((1950-y)-1.03t)/8274}$$
 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:

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

Appendix 4

Water composition, compilation of basic water analysis data

Idcode	Secup m	Seclow m	Sample no	Date	Charge Bal %	Na mg/L	K mg/L	Ca mg/L	Mg mg/L	HCO3- mg/L	Cl- mg/L	SO42- mg/L	SO4-S mg/L	Br- mg/l	F- mg/L	Si mg/L	Li mg/L	Sr mg/L	pH	EICond mS/m	Drill Water %	I- mg/L	
KFM07A	0	50	8810	2005-03-09	3.2	926	20.9	436	90.7	243	1,930	266	115	7.82	1.21	4.79	0.026	2.37	7.49	650	40	0.022	
KFM07A	50	100	8811	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	40	-
KFM07A	100	200	8812	2005-03-09	1.3	1,440	32.9	791	150	182	3,550	404	146	14.2	1.4	4.97	0.045	5.57	7.31	1,160	32	0.036	
KFM07A	200	250	8813	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	24	-
KFM07A	250	300	8814	2005-03-09	-0.7	1,740	39.3	1,080	184	115	4,780	495	177	19.7	1.2	4.70	0.053	8.65	7.03	1,450	22	0.048	
KFM07A	300	350	8815	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	20	-
KFM07A	350	400	8816	2005-03-09	1.4	1,940	33.0	2,100	137	57.0	6,600	397	138	49.0	1.17	3.10	0.058	21.3	6.60	1,990	15	0.123	
KFM07A	400	450	8817	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	9	-
KFM07A	450	550	8818	2005-03-09	-0.4	2,840	15.3	5,150	34.5	12.4	1,3600	130	48.1	132	1.18	1.13	0.06	61.1	6.46	3,460	3	0.340	
KFM07A	550	600	8819	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-
KFM07A	600	650	8820	2005-03-09	-0.4	2,870	13.7	5,420	23.3	11.8	14,100	109	39.9	139	1.31	1.28	0.067	66.4	6.89	3,570	2	0.356	
KFM07A	650	700	8821	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-
KFM07A	700	750	8822	2005-03-09	-0.8	2,890	13.6	5,450	22.3	13.2	14,300	106	39.2	149	1.32	1.49	0.062	64.7	6.99	3,560	2	0.393	
KFM07A	750	800	8823	2005-03-09	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2	-
KFM07A	800	850	8824	2005-03-09	-0.3	2,920	12.6	5,510	20.6	12.5	14,300	99.6	37.8	140	1.26	2.83	0.067	67.7	7.44	3,580	1	0.369	

- = Not analysed

A = results will be reported later

xx = No result due to analytical problems

* = Result not in SICADA

< "value" = below reporting limit or detection limit

ChargeBal % = Relative charge balance error %

SICADA: water_composition

Appendix 5

Isotopes, compilation of H-, O-, B-, S-, Cl-, Sr- and C-isotopes

Idcode	Secup m	Seclow m	Sample no	Date	Time	d2H dev SMOW	3H TU	d18O dev SMOW	10B/11B no unit	d34S dev CDT	d37Cl dev SMOC	87Sr/86Sr no unit	d13C dev PDB	14C pmC
KFM07A	350	400	8816	2005-03-09		-74.6	A	-9.0	A	-	A	0.719146	A	A
KFM07A	450	550	8818	2005-03-09		-85.0	A	-12.4	A	22.4	A	0.717914	A	A
KFM07A	600	650	8820	2005-03-09		-86.3	A	-12.8	A	-	A	0.717859	A	A
KFM07A	700	750	8822	2005-03-09		-89.5	A	-12.7	A	-	A	0.717858	A	A
KFM07A	800	850	8824	2005-03-09		-89.7	A	-12.9	A	-	A	0.717850	A	A

- = Not analysed

A = results will be reported later

xx = No result due to analytical problems

* = Result not in SICADA

< "value" = below reporting limit or detection limit

ChargeBal % = Relative charge balance error %

SICADA: water_composition