

Forsmark site investigation

Hydrochemical sampling and analyses in KFM12A

Results from two investigated borehole sections, 343.0–363.0 m and 516.0–536.0 m

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December 2007

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Abstract

Groundwater samples have been collected from two borehole sections, 343.0–363.0 m and 516.0–536.0 m, in borehole KFM12A. The sampling was conducted in connection to injection tests, using hydrotest equipment (PSS3) and the water was analysed according to SKB class 2, class 3 and class 5 respectively.

The water composition in section 343.0–363 m was stable during the pumping and sampling period. The same is true for the two samples from section 516.0–536.0 m. The chloride concentration in section 343.0–363.0 m amounted to 3,360 mg/L but the water samples were somewhat diluted by the flushing water (flushing water contents 9.9%). At 516.0–536.0 m the chloride concentration was 6,130 mg/L and the flushing water contents was as low as 0.5%, i.e. well within the acceptable limit. Furthermore, the water composition in the deep section reveals a rather clear Littorina sea water component while the marine signature of the groundwater from the upper section is very weak.

Sammanfattning

Provtagning av grundvatten har genomförts i två borrhålssektioner, 343,0–363,0 m och 516,0–536,0 m, i borrhål KFM12A. Provtagningen genomfördes i samband med injektionstester utförda med utrustning för hydrotester (PSS3). Vattenproverna analyserades enligt SKB's kemiklasser 2, 3 respektive 5.

Vattensammansättningen i sektion 343,0–363,0 m var stabil under hal pump- och provtagningsperioden. Det samma kan sägas för de två proverna som togs i sektion 516,0–536,0 m. Koncentrationen av klorid i sektion 343,0–363,0 m uppgick till 3 360 mg/L, dock var dessa prover något utspädda av spolvatten (spolvattenkoncentration 9,9 %). Vid 516,0–536,0 m var kloridkoncentrationen 6 130 mg/L och spolvattenhalten så låg som 0,5 % vilket är väl inom den acceptabla nivån. Vidare visar sammansättningen i den djupare sektionen ganska klart på ett vatten med ursprung från Littorinahavet medan den marina signaturen i grundvattnet från den övre sektionen är mycket svag.

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1 Introduction

This document reports performance and results from groundwater sampling and analyses in borehole KFM12A within the site investigation programme at Forsmark /1/. The investigation was carried out according to the method “Simple water sampling in percussion and core drilled boreholes” in connection to injection tests. The hydrotest equipment (PSS3) was used for delimiting the sections and pumping of water and the work was carried out in accordance with activity plan AP PF 400-07-023. The controlling documents for performing this activity are listed in Table 1-1. Both activity plan and method documents are SKB’s internal controlling documents. The field work was performed in May 2007.

Original data from the reported activity are stored in the primary database Sicada. Data are traceable in Sicada by the activity plan number (AP PF 400-07-023). Only data in databases are accepted for further interpretation and modelling. The data presented in this report are regarded as copies of the original data. Data in the database may be revised, if needed. However, such revision of the database will not necessarily result in a revision of this report although the normal procedure is that major data revisions entail a reversion of the P-report. Minor revisions are normally presented as supplements, available at www.skb.se.

Borehole KFM12A is a telescopic borehole /2/ and its location together with two percussion drilled boreholes at the drill site (DS12) /3/ are shown in Figure 1-1. KFM12A is inclined at 61° with a northeast bearing. The borehole section between 0–59.75 m is percussion drilled and has a stainless steel casing with an internal diameter of 200 mm, whereas the 59.75–601.04 m interval is core drilled with a diameter of 77.3 mm. The design of the borehole is presented in Appendix 1. The borehole was designed and treated as a so-called SKB chemical-type borehole; see the SKB method descriptions MD 620.003 (Method description for drilling cored boreholes) and MD 610.003 (Method description for percussion drilling). An SKB chemical-type borehole requires cleaning procedures to be carried out on all equipment used in the borehole, both during and after drilling, according to level 2 in the cleaning instructions outlined in MD 600.004. Initially, KFM12A was not planned to be a chemical type of borehole, but since it came to be a telescopic borehole and the routines were well established, generally the same procedure as for a chemical borehole was applied.

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

Activity plan	Number	Version
Hydraulic injection tests in borehole KFM12A with PSS3.	AP PF 400-07-023	1.0
Measurement system descriptions	Number	Version
Pipe String System	SKB MD 345.100-124	–
Metodbeskrivning för enkel vattenprovtagning i hammarborrhål och kärnborrhål.	SKB MD 423.002	2.0
Instruktion för rengöring av borrhålls- och viss markbaserad utrustning.	SKB MD 600.004	1.0
Provtagning och analys-kemilaboratorium.	SKB MD 452.001-019	–

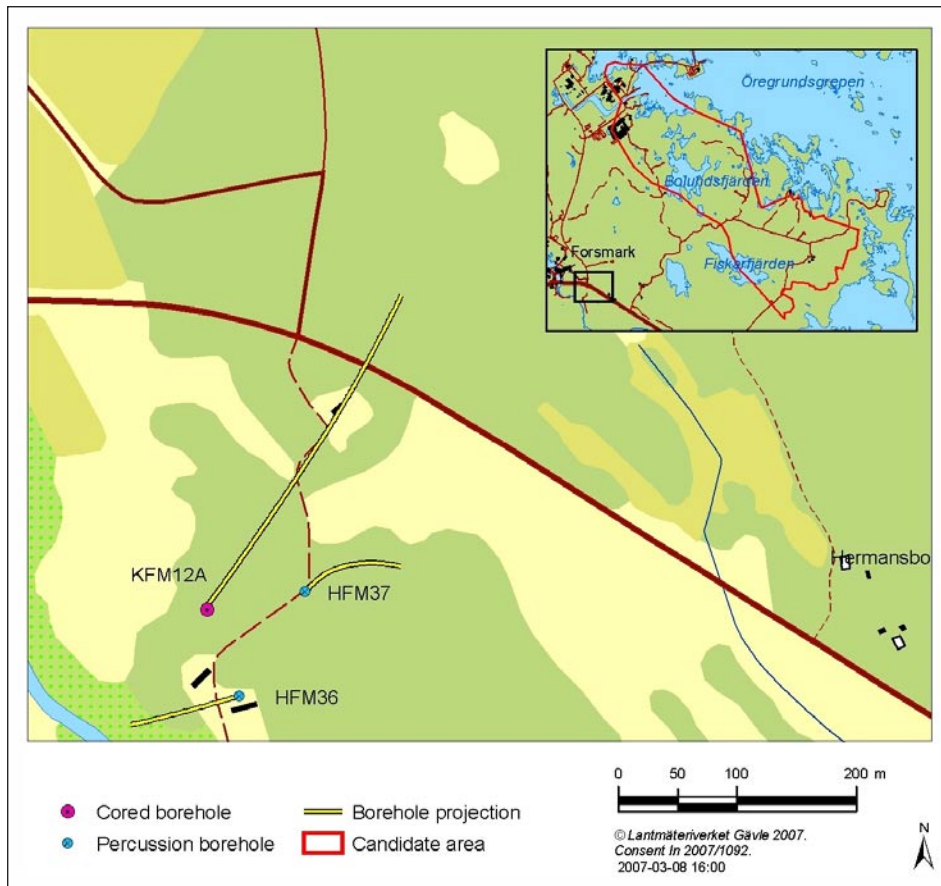


Figure 1-1. Drill site DS12 with locations and projections on the horizontal plane of the current boreholes. At the top right corner, the investigation area at Forsmark (approximately the area shown) with the candidate area selected for more detailed investigation in red outlier (DS12 the black square).

2 Objective and scope

Hydrochemical information from borehole KFM12A was considered to be somewhat less important for the hydrogeochemical model compared to studies in boreholes within the target area or close to the target area, /4/. Yet, it was desirable to obtain a general idea about the groundwater composition also from the distant Forsmark zone area. This condition, together with time constraints and the fact that the mobile chemical equipment was occupied at investigations in boreholes KFM11A and KFM08D, were the reasons for using hydrotest equipment (PSS3) for the chemical investigation (delimiting of borehole sections and pumping of groundwater) in KFM12A. The high capacity of the pump in PSS3, which allows a high pumping flow rate, was favourable also from a flushing water point of view.

The analytical programme was carried out according to SKB chemistry class 2 and 3 in the shallow section (343.0–363.0 m) and class 5 in the deeper section (516.0–536.0 m) /1/.

3 Background

3.1 Flushing water history

The percussion drilled borehole HFM36 /3/ served as a supply well for the flushing water used to drill borehole KFM12A and the chemical composition of the flushing water was checked three times before use /5/ and twice during core drilling /2/. The flushing water showed a rather shallow groundwater character, and accordingly the concentrations of e.g. sodium, calcium, chloride and bromide were lower and the alkalinity was higher than in groundwater from the two investigated sections in KFM12A. The core drilling of the 601.04 m long borehole consumed 483 m³ of flushing water and the volume of returned water pumped from the borehole by air-lift pumping during drilling was 543 m³.

Automatic dosing equipment for injection of Uranine was installed in the water line that supplied flushing water to the drilling head. The Uranine concentration in the flushing water and returned water was checked regularly and a total of 58 samples of each sample type were analysed. The Uranine concentrations in the flushing water and in the returned water are presented in Figure 3-1. A water budget, presenting the amount of Uranine added to the borehole via the flushing water and the estimated amount recovered in the return water, is given in Table 3-1. The table clearly demonstrates that some amounts of flushing water remains in the aquifer after completed drilling.

Table 3-1. Uranine addition to KFM12A via flushing water during core drilling and the amount recovered by the air-lift pumping.

Uranine	(g)
Added, according to the log book.	98
Added, calculated from the average Uranine concentration and the total volume of flushing water.	80
Recovered, estimated from the average Uranine concentration and the total volume of returned water.	61

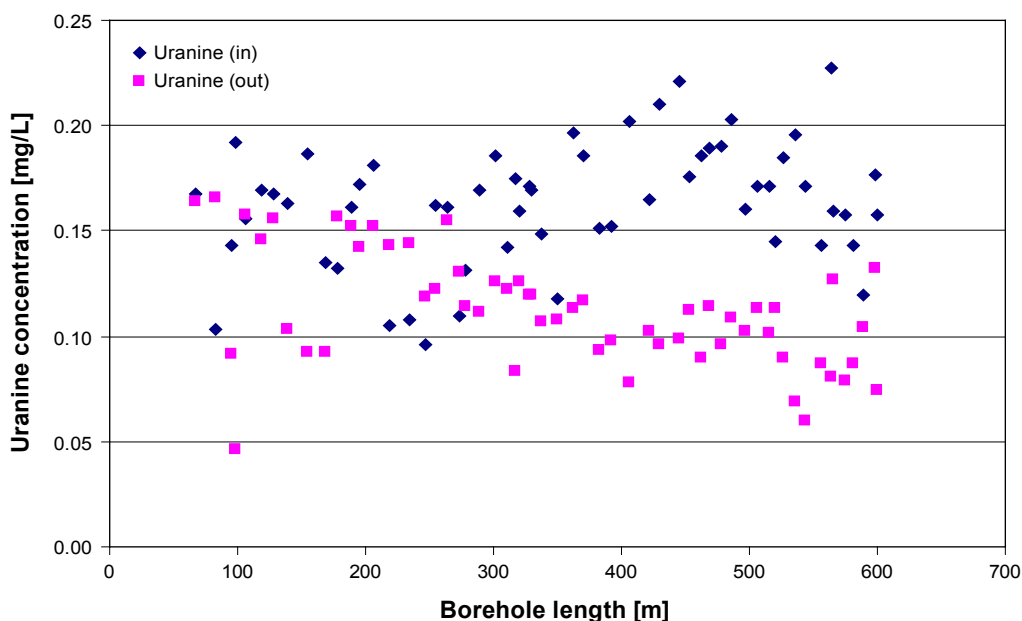


Figure 3-1. Uranine concentrations in the flushing water and in the recovered water versus borehole length.

3.2 Previous events and activities in the borehole

Although KFM12A was designed and drilled as an SKB chemical-type core borehole and thus suited for hydrochemical characterisation, this was not the primary purpose and some of the SKB chemical type routines were not followed. No differential flow logging was conducted in this borehole and results from preceding injection tests were used in order to select suitable borehole sections for hydrochemical sampling. Injection tests belong to the type of activities that may contaminate subsequent groundwater samples and are normally performed after hydrochemical investigations. The activities performed in KFM12A prior to the chemistry campaign are listed in Table 3-2 below.

3.3 Choice of borehole sections

The preceding injection tests displayed several highly water bearing fractures/fracture zones in the borehole /8/. The deepest flow anomaly with a sufficiently high transmissivity to allow pumping with the PSS3-pump was selected, first because it represents repository depth and secondly, because of the higher probability to obtain samples with a low flushing water content close to the bottom of the borehole. A complementary, more shallow section with a suitable transmissivity was selected at some distance from the deep section (343.0–363.0 m borehole length), see Figure 3-2 and Table 3-3. Flow anomalies with very high hydraulic transmissivity were avoided due to expected problems with flushing water contamination.

Table 3-2. Activities performed in KFM12A prior to and in connection with the chemical characterisation.

Activities performed	Date of completion	Section (m borehole length)	Comment
Percussion drilling	2006-09-18	0–59.75	
Core drilling	2007-03-12	59.75–601.04	HFM36 was the source of flushing water for drilling the cored part of KFM12A /2/. Flushing water volume = 483 m ³ . Return water volume 543 m ³ .
Geophysical logging	2007-03-22	60–585	/6/
BIPS-logging	2007-03-21	61–598	/7/
Injection tests	2007-04-24	63–596	/8/

Table 3-3. Selected borehole sections for hydrochemical sampling with hydraulic transmissivity values calculated from injection tests (T_t).

Section (m)	Elevation mid sect. (m.b.s.l.)	T_t (m ² /s) /8/	Comments
343.0–363.0	294	6.6E–7	The highly transmissive flow anomalies in the vicinity were avoided due to risk for high flushing water content.
516.0–536.0	439	2.7E–7	

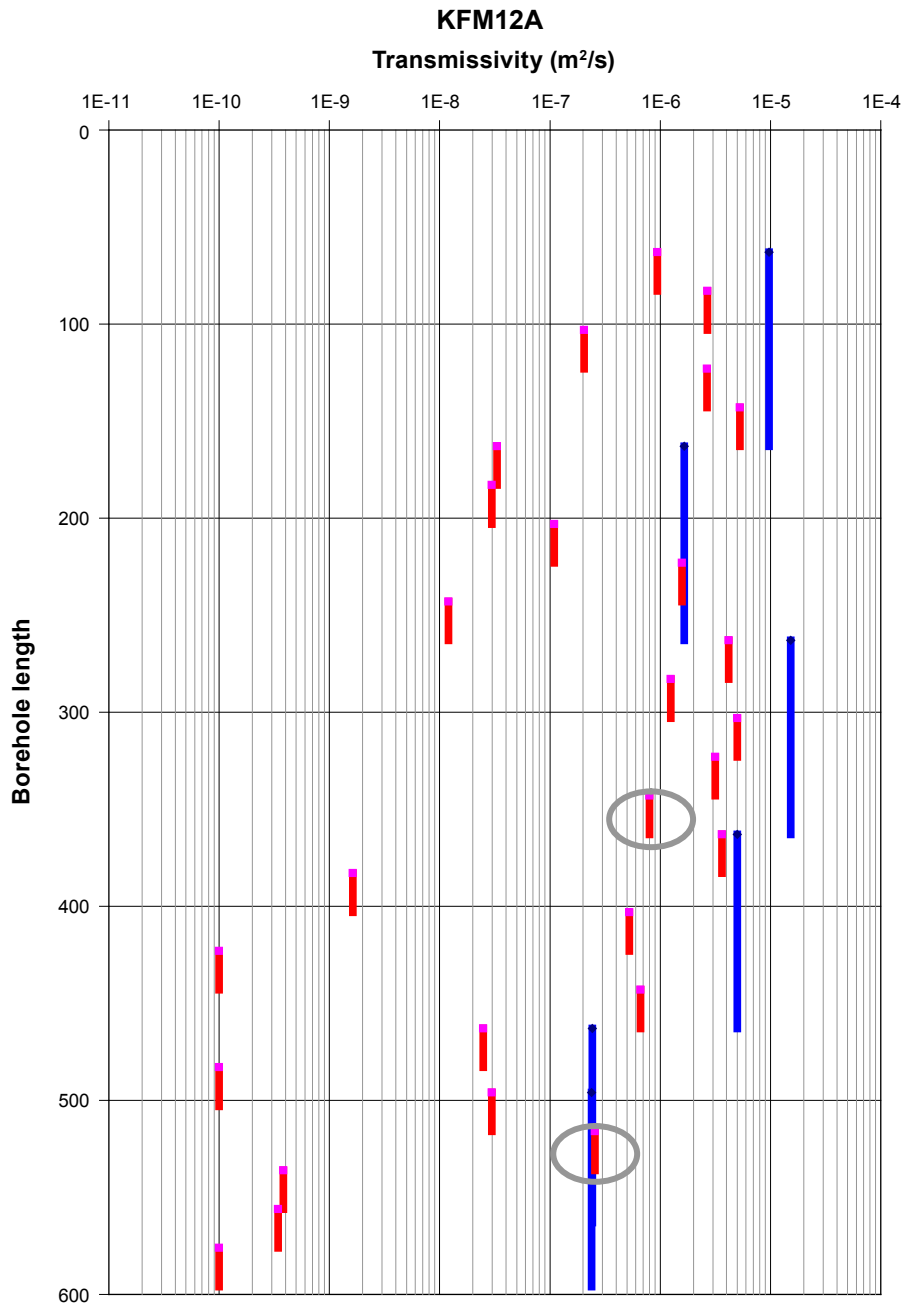


Figure 3-2. Transmissivities along borehole KFM12A. The two flow anomalies selected for hydrochemical sampling are marked as grey ovals.

4 Equipment

4.1 The Pipe String System (PSS)

The SKB pipe string system (PSS) consists of a measurement container and a set-up of downhole equipment. The system is normally used for hydraulic pumping tests and hydraulic injection tests but was in this case applied for pumping and chemical sampling. The equipment is described in SKB MD 345.100-124 (Pipe String System, SKB internal controlling document).

The PSS equipment is designed for flow rates between 5 and 30–40 L/min. In order to pump at lower flow rates (down to 1 L/min), it is necessary to re-circulate the pumped water back to the borehole.

The hydrotest unit PSS3 in combination with the laboratory unit L3 for analytical work were used in borehole KFM12A. However, the laboratory unit was not placed at the drill site and thus not directly connected to the outlet of the pumped water during pumping.

4.1.1 Measurement container

The PSS is primarily designed for pumping and injection tests in borehole sections isolated from the remaining borehole by a double packer system. All equipment needed to perform the tests is located in a steel container placed on pallets to adjust to a suitable working level in relation to the borehole casing. The container is divided into a data and a workshop compartment, see Figure 4-1.

The hoisting rig is of a hydraulically chain-feed type in which the jaws, holding the pipe string, are opened hydraulically and closed mechanically by springs. The rig is equipped with a load transmitter, maximum 22 kN, and a limiting value for the load may be adjusted.

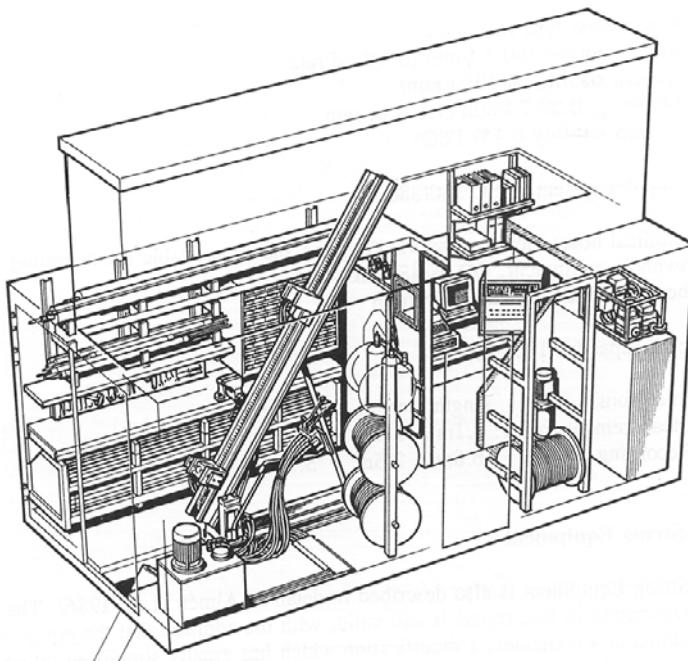


Figure 4-1. Outline of the PSS3 container with equipment.

The packers and the test valve are operated hydraulically by water filled pressure vessels. Expansion and release of packers as well as opening and closing of the test valve is handled by magnetic valves controlled by the software in the data acquisition system.

4.1.2 Downhole equipment

A schematic drawing of the downhole equipment is shown in Figure 4-2. The pipe string consists of aluminium pipes 3 m in length with an inner diameter of 21 mm connected by stainless steel taps sealed with double o-rings. The length of the test section comprises pipes of 5 m length, the number of which can be varied to investigate 5, 20 or 100 m sections, and the electric cable is also prepared for these lengths. Figure 4-3 shows lowering of the pipes into the borehole. Pressure is measured above, within and below the test section, which is isolated by two packers. The groundwater temperature in the test section is also measured. The hydraulic connection between the pipe string and the test section can be closed or opened by a test valve operated by the measurement system.

At the lower end of the borehole equipment, a level indicator (caliper type) gives a signal when the reference length marks, which are milled into the borehole wall at regular distances along the borehole, are passed.

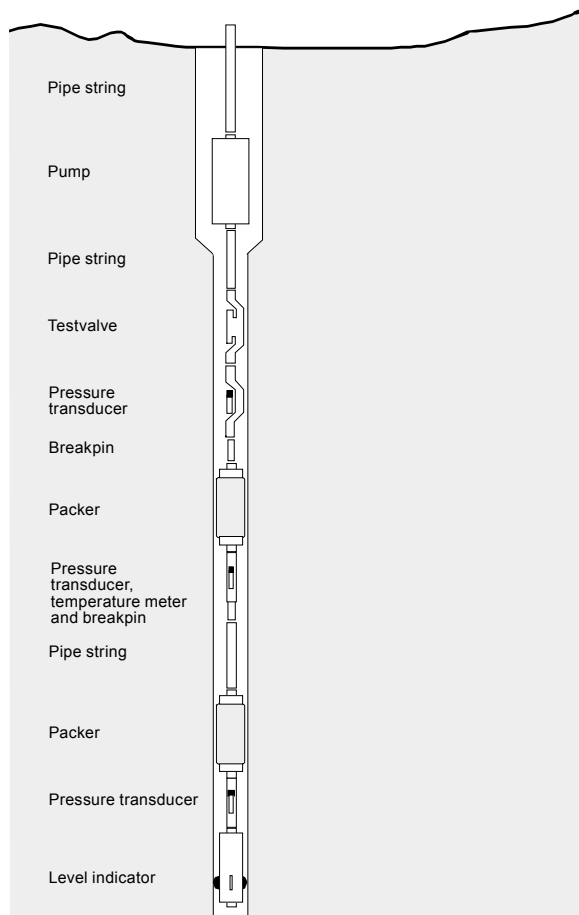


Figure 4-2. Schematic drawing of the downhole equipment in the PSS3 system.



Figure 4-3. Lowering of aluminium-pipes into the borehole during pumping with PSS3.

5 Performance

5.1 General

Chemical characterisation in borehole KFM12A was conducted according to activity plan AP PF 400-07-023 following the method described in SKB MD 423.002. Two sections were sampled, 343.0–363.0 m and 516.0–536.0 m, respectively.

5.2 Water sampling

Prior to the first sampling, the water volume in each section was exchanged at least three times to obtain representative water samples. Four groundwater samples were collected from section 343.0–363.0 m during a period of two weeks. Only the last sample was fully analysed (SKB class 3) due to high flushing water content in the previous samples. From section 516.0–536.0 m two SKB class 5 samples were collected with a gap of six days in between.

Sample portions intended for analysis of major constituents and trace metals (by ICP technique), DOC and iron (by spectrometry) were filtered on-line or by using a syringe. Disposable 0.40 µm filters were fitted directly to the 4/6 mm polyamide-tube leading the pumped water from the borehole section or to the tip of the syringe. During the entire sampling, laboratory gloves were used to minimize the risk of contaminating the samples.

5.2.1 Water sampling in section 343.0–363.0 m

The chemical characterisation in section 343.0–363.0 m was performed with a pumping flow rate of about 1.5 L/min and a drawdown of approximately 30 m. The events during the investigation are listed in Table 5-1. A total volume of approximately 22 m³ water was extracted from the section during the pumping period.

5.2.2 Water sampling in section 516.0–536.0 m

The chemical characterisation in section 516.0–536.0 m was performed with a pumping flow rate of about 40 mL/min and a drawdown of approximately 40 m. The events during the investigation are listed in Table 5-2. A total volume of approximately 0.4 m³ water was extracted from the section during the pumping period.

Table 5-1. Events during pumping with Pipe String System in section 343.0–363.0 m.

070425	Pump start
070426	Water sampling: SKB class 2
	Pump failure
070427	Restart of pump
	Pump failure
070430	Restart of pump after failure
070504	Water sampling: SKB class 2
070509	Water sampling: SKB class 2
070510	Water sampling: SKB class 3
070513	Pump stop

Table 5-2. Events during pumping with Pipe String System in section 516.0–536.0 m.

070514	Pump start
070515	Water sampling: SKB class 5
070521	Water sampling: SKB class 5 with all options
070521	Pump stop

5.3 Water sample treatment and analyses

A water sample is defined as groundwater collected during one day and consists of several sample portions, labelled with the same sample number.

An overview of sample treatment and analysis routines for major constituents, minor anions, trace metals and isotopes is given in Appendix 2. The routines are applicable independently of sampling method or sampling object.

6 Nonconformities

The flushing water content in the groundwater from section 343.0–363.0 m did not reach below 1%, which is the upper limit for a fully representative sample, within the pumping period. The flushing water content in the last sample measured 9.9%.

7 Data handling and interpretation

7.1 Water analysis data

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

Several 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 $\pm 5\%$ are considered acceptable.

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

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

All results from special analyses of **trace metals** and **isotopes** are inserted directly into primary data tables. In cases where the analyses are repeated or performed by more than one laboratory, a “best choice” notation will indicate those results which are considered most reliable.

An overview of the data management is given in Figure 7-1.

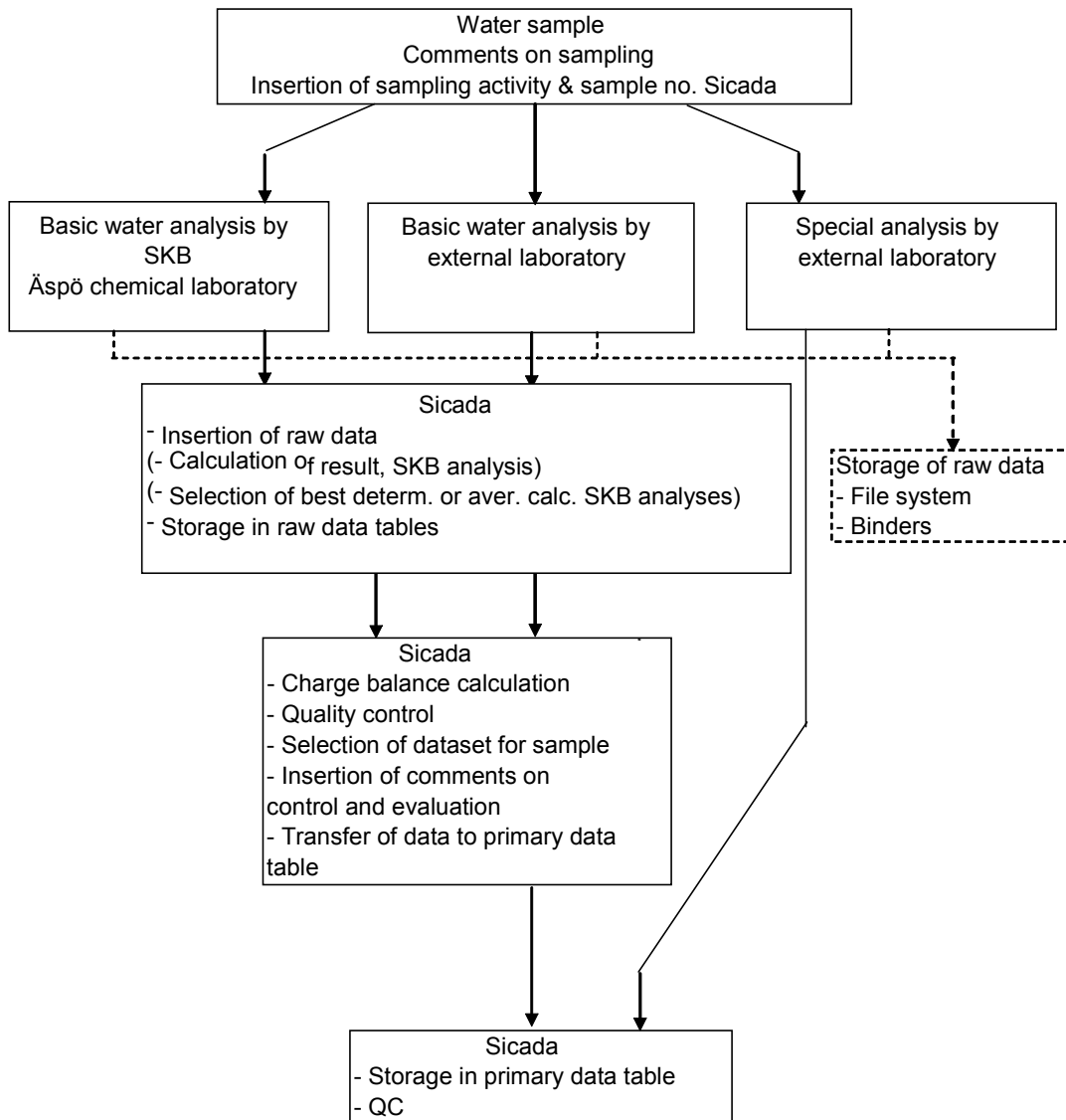


Figure 7-1. Overview of data management for hydrogeochemical data.

8 Results

8.2 Water analysis

8.2.1 Basic water analyses

The basic analyses include the major constituents Na, K, Ca, Mg, Fe, Li, Mn, S, Sr, SO_4^{2-} , Cl^- , Si, HCO_3^- , Br^- and F^- . Samples collected according to SKB chemistry class 5 include also P, I⁻, HS^- , NH_4^+ , NO_2^- , NO_3^- , TOC and DOC. Furthermore, measurement of pH and electrical conductivity (EC) are included. Another important parameter is the flushing water content in each sample.

The charge balance errors did not exceed the acceptable limit of $\pm 5\%$ in any of the samples. The basic water analysis data and relative charge balance errors are compiled in Appendix 3, Table A3-1.

The flushing water contents in the sample series collected from the two borehole sections are presented in Figure 8-1. The contents should not exceed 1% in order for a sample to be considered representative for the groundwater of the sampled fracture. This condition was met for section 516.0–536.0 m (0.5%) but not for section 343.0–363.0 m (9.9%). The percentage of flushing water in the samples was calculated using the Uranine concentration of the groundwater samples in relation to the average Uranine concentration (0.170 mg/L) from the flushing water samples collected during drilling.

The groundwater samples from both sections showed reasonably stable chloride concentrations. However, the number of samples was small. The chloride concentrations are plotted versus the corresponding electrical conductivity values in Figure 8-2. The plot gives a rough check of both the measured EC values and the chloride concentrations. As shown, the data from the two investigated sections in KFM12A agree well with the regression line obtained by previous data from the site investigation at Forsmark.

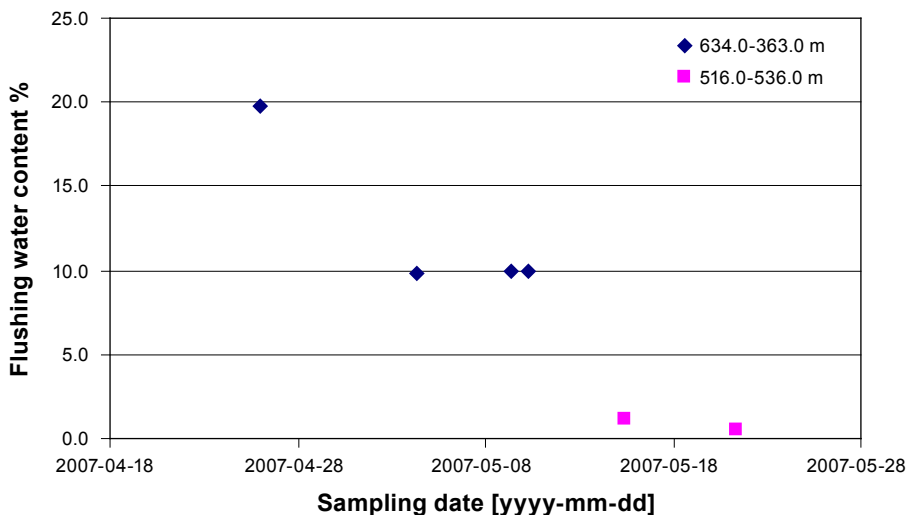


Figure 8-1. Flushing water contents in the groundwater samples from the two sections sampled in KFM12A.

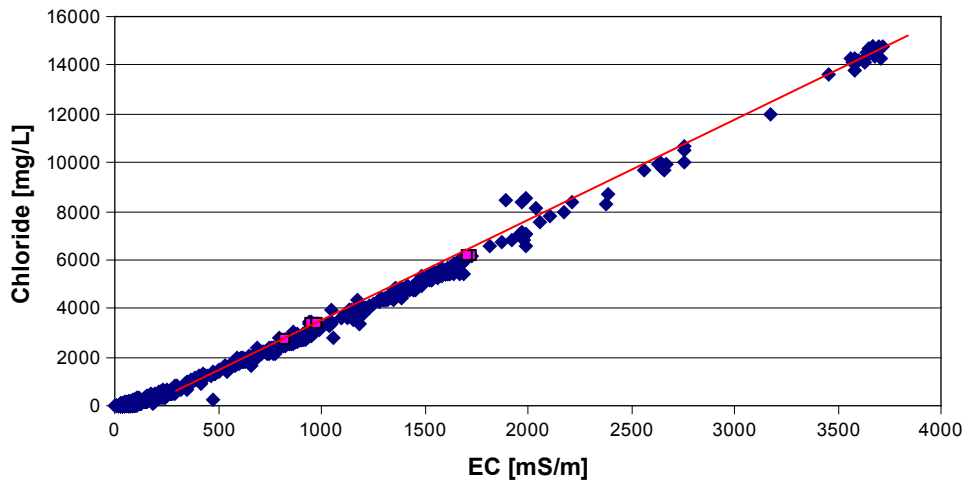


Figure 8-2. Chloride concentration versus electrical conductivity. Data from previous investigations at Forsmark are used to show the linear trend. Data from KFM12A are shown in pink.

8.2.2 Trace elements (rare earth metals and others)

The two samples collected in section 516.0–536.0 were analysed for trace elements. The analyses of trace and rare earth metals include Al, B, Ba, U, Th, Sc, Rb, Y, Zr, In, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu. Commonly occurring metals, such as Cu, Zn, Pb and Mo, are not included in the analysis programme due to contamination considerations. The risk of contamination is large also for aluminium but the aluminium concentration is generally still reported due to its importance for the modelling work. In this case both samples show high Al concentrations (23 and 102 µg/L) and are most probably contaminated by the pipe string made of aluminium. The trace element data are compiled in Appendix 3, Table A3-2.

8.2.3 Stable and radioactive isotopes

The SKB class 3 groundwater sample from borehole section 343.0–363.0 included the isotopes $\delta^2\text{H}$, $\delta^{18}\text{O}$ and ^3H (TU) and the two SKB class 5 samples from the deep section included also $^{10}\text{B}/^{11}\text{B}$, $\delta^{34}\text{S}$, $\delta^{13}\text{C}$, $^{87}\text{Sr}/^{86}\text{Sr}$, ^{14}C (pmC), ^{238}U , ^{234}U , ^{230}Th , ^{226}Ra and ^{222}Rn .

Available isotope data at the time of reporting are compiled in Appendix 3, Table A3-3 and A3-4. The $\delta^{18}\text{O}$ signature in groundwater from 343.0–363.0 m indicates presence of a strong glacial meltwater component. The glacial meltwater character in section 516.0–536.0 m is less clear. For sample 12792, recalculation of $^{238}\text{U} = 37 \text{ mBq/L}$ gives $U = 2.98 \text{ µg/L}$ which agrees very well with the result from the ICP MS determination ($U = 2.99 \text{ µg/L}$).

9 Summary and discussions

The hydrochemical investigation in the most distant borehole KFM12A outside the candidate area at Forsmark was less extensive compared to investigations performed in previous core drilled boreholes within the candidate area. No on-line measurements of pH, Eh, EC, O₂ and temperature were conducted. Furthermore, only a few samples were collected from each section and the number of analysed constituents was reduced. Figure 9-1 displays chloride concentrations versus depth and Figure 9-2 shows magnesium concentrations versus chloride concentrations for KFM12A together with corresponding data from other boreholes at Forsmark.

The main conclusions from the results of the chemical sampling in KFM12A are:

- The chloride and magnesium concentrations in the deep section indicate presence of a Littorina sea water component while the marine character of the groundwater from the upper section is much weaker.
- The investigation in section 516.0–536.0 m borehole length was successful as the last sample showed a flushing water content below 1% which is the upper limit for a fully representative sample. The flushing water contents in section 343.0–363.0 m did not reach below 9.9% in spite of the prolonged pumping period, and the results from this section are of limited use for hydrochemical modelling.
- The quality of the water analyses is generally high, based on comparison between results from different methods and the fact that all samples showed acceptable charge balance errors within $\pm 5\%$.
- The groundwater from the shallow borehole section at 343.0–363.0 m borehole length showed an unusually low $\delta^{18}\text{O}$ value indicating presence of water with a glacial meltwater origin.
- The uranium concentration in the deep section is reasonably low (2.99 $\mu\text{g/L}$), which is far from the surprisingly high concentrations measured in some of the borehole sections in Forsmark (up to 120 $\mu\text{g/L}$).

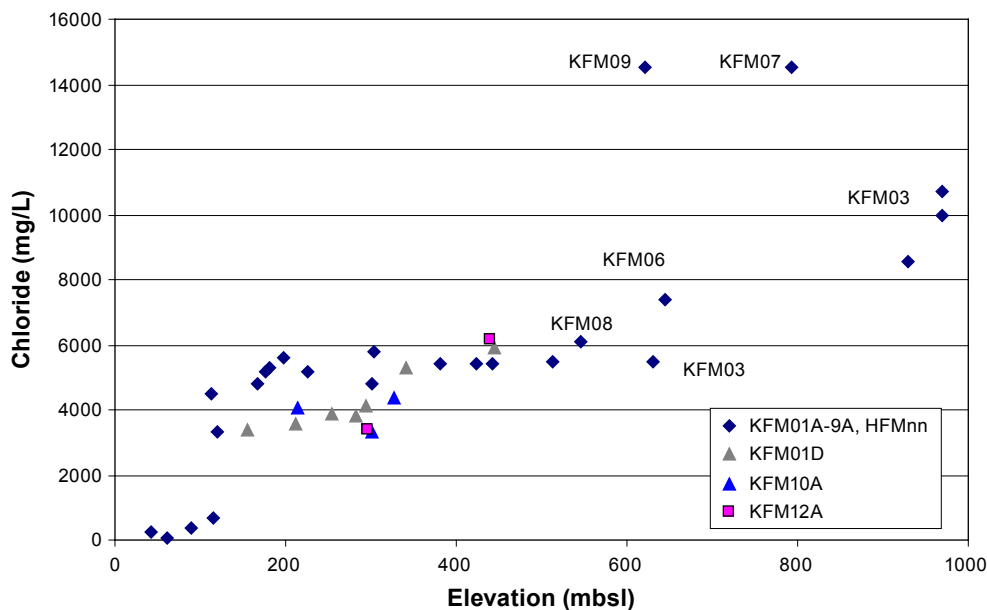


Figure 9-1. Chloride concentrations versus depth (m) at the Forsmark site.

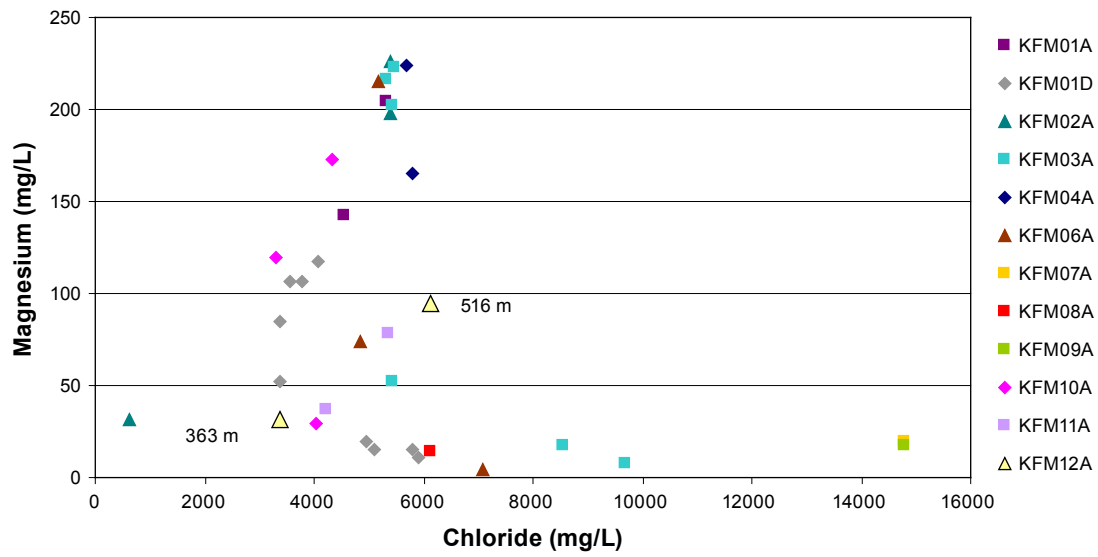


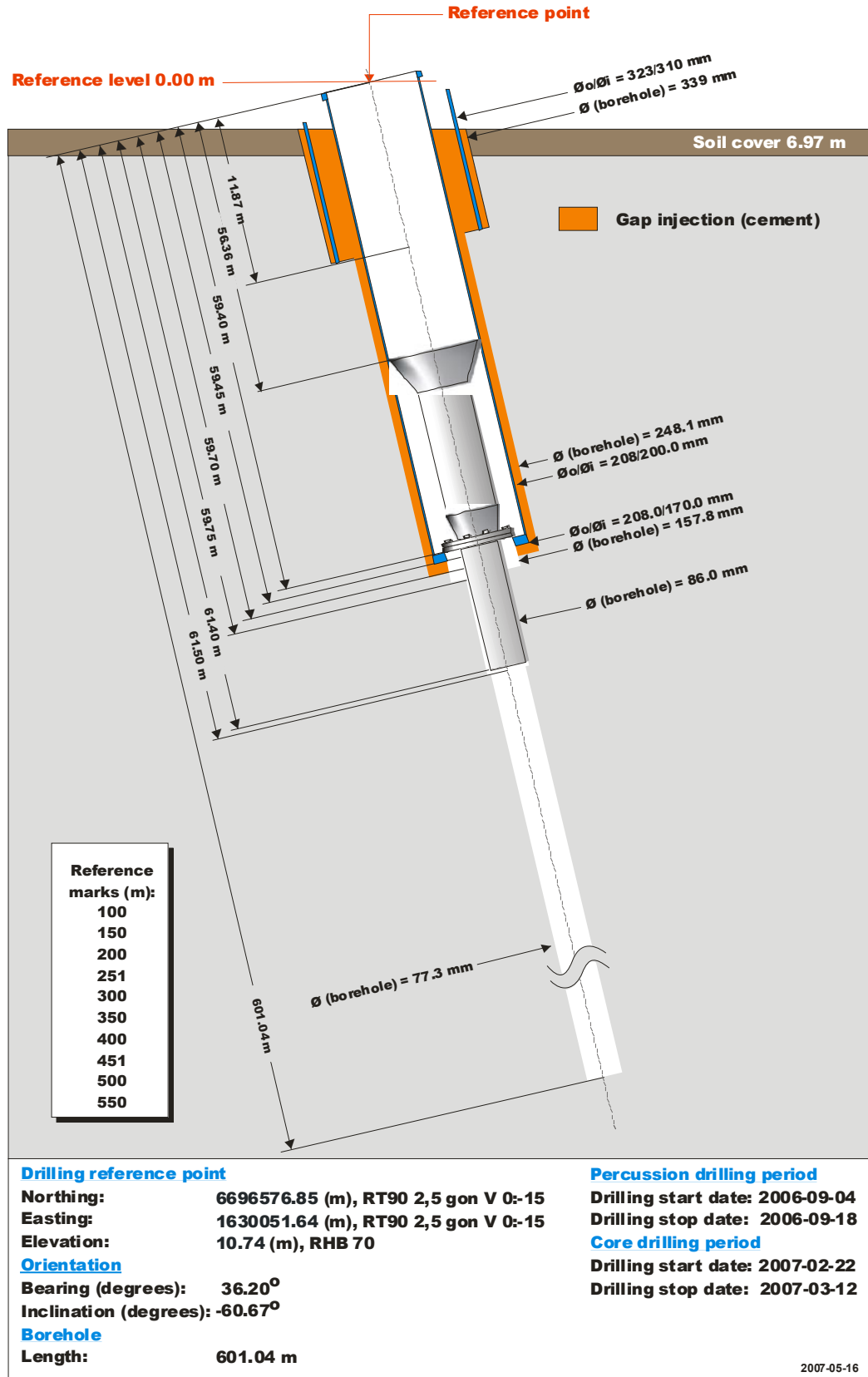
Figure 9-2. Magnesium concentrations versus chloride concentrations at the Forsmark site.

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Design of cored borehole KFM12A

Technical data
Borehole KFM12A



Sampling and analytical methods

Table A2-1. 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.
Anions 1.	HCO ₃ pH(lab) cond (lab)	Plastic	250	No	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 (1 mL 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	Yes	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, Ti, 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)
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

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 analyser Shimadzu TOC5000	Short transportation time
Environmental isotopes	$\delta^2\text{H}$, $\delta^{18}\text{O}$	Plastic	100	No	–	MS	Not critical (month)
Tritium	^3H (enhanced.)	Plastic (dry bottle)	500	No	–	LSC	–
Chlorine-37	^{37}Cl	Plastic	100	No	–	ICP MS	Not critical (month)
Carbon isotopes	^{13}C , pmC	Plastic (HDPE)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	^{34}S	Plastic	500–1,000	No	–	Combustion, ICP MS	No limit
Strontium-isotopes	$^{87}\text{Sr}/^{86}\text{Sr}$	Plastic	100	No	–	TIMS	Days or Week
Uranium and Thorium isotopes	^{234}U , ^{235}U , ^{238}U , ^{232}Th , ^{230}Th ,	Plastic	50 1,000	No	–	Chemical separat. Alfa/gamma spectrometry	No limit
Boron isotopes	$^{10}\text{B}/^{11}\text{B}$	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP – MS	No limit
Radon and Radium isotopes	^{222}Rn , ^{226}Ra	Plastic	500–1,000	No	No	LSS	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 stain-less 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	–	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
Carbon isotopes in humic and fulvic acids	^{13}C , ^{14}C (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	No	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
LSS	Liquid Scintillation Spectrometry
(A)MS	(Accelerator) Mass Spectrometry
GC	Gas Chromatography

Table A2-2. 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 ⁻	Mohr- titration	> 70	mg/L	5%	<10%
Cl ⁻	IC	1 – 100		6%	10%
SO ₄	IC	1	mg/L	10%	15%
Br ⁻	IC	0.2	mg/L	9%	20%
Br ⁻	ICP	0.001		15%	
F ⁻	IC	0.1	mg/L	10%	20%
F ⁻	Potentiometric	–		–	
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 50 (SKB)	µg/L	0.8 (0.8–20 µg/L) 5% (> 20 µg/L) 20%	20%
PO ₄ as P	Spectrophotometry	0.7	µg/L	0.7 (0.7–20 µg/L) 3% (> 20 µg/L)	20%

Component	Method	Reporting limits or range		Unit	Measurement uncertainty ³	"Total" uncertainty ⁴
SiO ₄	Spectrophotometry	1		µg/L	3% (>200 µg/L)	–
O ₂	Iodometric 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	ICP	0.01		µg/L	20%	Correct order of size (low conc.)
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 ² H	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	–	–
234U, 235U, 238U, 232Th, 230Th	Alfa spectr.	0.0005		Bq/L ¹²	5%	–
222Rn, 226Rn	LSS	0.03		Bq/L	5%	–

1. Reporting limits at salinity $\leq 0.4\%$ (520 mS/m) and $\leq 3.5\%$ (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 deviation¹³ 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 deviation¹³ from SMOC (Standard Mean Oceanic Chloride).
8. Per mille deviation¹³ from PDB (the standard PeeDee Belemnite).
9. 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.
10. Per mille deviation¹³ 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/kg²³⁸U ppm Th = 3.93 Bq/kg²³²Th
13. 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.

Compilation of water analysis data

Table A3-1. Water composition.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	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	SO ₄ _S mg/L	Br mg/L	F ⁻ mg/L	Si mg/L	Fe mg/L	Fe-tot mg/L	Fell mg/L	Mn mg/L
KFM12A	343	363	12723	2007-04-26	-	-	-	-	-	59	2,740	-	-	-	-	-	-	-	-	-
KFM12A	343	363	12786	2007-05-04	-	-	-	-	-	39.9	3,360	-	-	-	-	-	-	-	-	-
KFM12A	343	363	12787	2007-05-09	-	-	-	-	-	41.0	3,360	-	-	-	-	-	-	-	-	-
KFM12A	343	363	12788	2007-05-10	-0.1	946	5.34	1,080	31.1	41.2	3,360	111	39.7	21.3	1.16	5.72	-	-	-	-
KFM12A	516	536	12791	2007-05-15	0.01	1,540	11.3	2,190	89.2	52.0	6,190	373	138	30	1.16	6.72	0.25	0.27	0.262	0.83
KFM12A	516	536	12792	2007-05-21	-0.78	1,570	11.5	2,070	94.1	58.9	6,130	381	140	28.7	1.32	7.64	0.268	0.291	0.276	0.859

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Li mg/L	Sr mg/L	I ⁻ mg/L	pH	DOC mg/L	TOC mg/L	HS ⁻ mg/L	Drill-water µg/L	EICond mS/m	NH ₄ N mg/L	NO ₂ N mg/L	NO ₃ N mg/L	NO ₂ N/NO ₃ N mg/L	PO ₄ P mg/L	P mg/L
KFM12A	343	363	12723	2007-04-26	-	-	-	7.73	-	-	-	19.8	825	-	-	-	-	-	-
KFM12A	343	363	12786	2007-05-04	-	-	-	7.81	-	-	-	9.8	956	-	-	-	-	-	-
KFM12A	343	363	12787	2007-05-09	-	-	-	7.74	-	-	-	9.9	978	-	-	-	-	-	-
KFM12A	343	363	12788	2007-05-10	0.036	14.2	-	7.79	-	-	-	9.9	982	-	-	-	-	-	-
KFM12A	516	536	12791	2007-05-15	0.05	26.2	0.084	7.41	1.9	-	0.023	1.2	1,730	0.176	<0.0002	0.0003	0.0004	<0.0005	<0.04
KFM12A	516	536	12792	2007-05-21	0.05	24.8	0.073	7.54	1.5	1.1	0.034	0.5	1,710	0.19	<0.0002	0.0004	0.0005	<0.0005	<0.04

-- = Not analysed

< "value" = result less than reporting limit

RCB % = Rel. charge balance error %

SICADA: water_composition

Table A3-2. Trace elements.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	U ug/L	Th ug/L	B ug/L	As ug/L	Sc ug/L	Cd ug/L	Hg ug/L	V ug/L	Rb ug/L	Y ug/L	Zr ug/L	In ug/L	Cs ug/L	Ba ug/L	La ug/L	Hf ug/L	Tl ug/L	Ce ug/L
KFM12A	516.00	536.00	12791	2007-05-15	4.74	<0.2	771.0	<1	<0.5	<0.002	0.393	27.9	0.92	<0.3	<0.5	0.818	116	0.172	<0.05	<0.05	<0.05	0.155
KFM12A	516.00	536.00	12792	2007-05-21	2.99	<0.2	762.0	<1	<0.5	<0.002	0.274	27.5	2.28	<0.3	<0.5	0.792	127	0.413	<0.05	<0.05	<0.05	0.461

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Pr ug/L	Nd ug/L	Sm ug/L	Eu ug/L	Gd ug/L	Tb ug/L	Dy ug/L	Ho ug/L	Er ug/L	Tm ug/L	Yb ug/L	Lu ug/L	Cr ug/L	Co ug/L	Ni ug/L	Sb ug/L	Al ug/L
KFM12A	516.00	536.00	12791	2007-05-15	<0.05	0.0894	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	0.427	<0.05	<0.05	0.277	23.2
KFM12A	516.00	536.00	12792	2007-05-21	0.05663	0.287	0.0535	<0.05	<0.05	<0.05	0.101	<0.05	0.0921	<0.05	0.0556	<0.05	0.77	0.0952	3.21	<0.1	102

- = Not analysed

< "value" = result less than reporting limit

SICADA: trace_elements_1, trace_elements_2

Table A3-3. Isotopes I (H-, O-, B-, S-, Cl- and C-isotopes).

Idcode	Secup m	Seclow m	Sample no.	Sampling date	δ²H dev SMOW	³H TU	δ¹⁸O dev SMOW	¹⁰B/¹¹B no unit
KFM12A	343.00	363.00	12788	2007-05-10	-118.7	<0.8	-15.6	-
KFM12A	516.00	536.00	12791	2007-05-15	-91.2	1.0	-12.1	0.2388
KFM12A	516.00	536.00	12792	2007-05-21	-89.9	<0.8	-11.7	0.2385

Idcode	Secup m	Seclow m	Sample no.	Sampling date	δ³⁴S dev CDT	δ¹³C dev PDB	⁸⁷Sr/⁸⁶Sr no unit	¹⁴C	δ³⁷Cl
KFM12A	343.00	363.00	12788	2007-05-10	-	-	-	-	-
KFM12A	516.00	536.00	12791	2007-05-15	24.0	-	0.716968	-	-
KFM12A	516.00	536.00	12792	2007-05-21	26.1	-12.44	0.716951	A	-0.23

- = Not analysed

A = results will be reported later

SICADA: isotopes_1

Table A3-4. Isotopes II (U-, Th, Ra- and Rn-isotopes).

Idcode	Secup m	Seclow m	Sample no.	Sampling date	²³⁸U mBq/L	²³⁵U mBq/L	²³⁴U mBq/L	²³⁰Th mBq/L
KFM12A	516.00	536.00	12792	2007-05-21	37	1.4	140	0.2

Idcode	Secup m	Seclow m	Sample no.	Sampling date	²³²Th mBq/L	²²⁶Ra Bq/L	²²²Rn Bq/L	²²²Rn corr Bq/L
KFM12A	516.00	536.00	12792	2007-05-21	0.2	<0.015	160	223

- = Not analysed

< "value" = result less than detection limit

SICADA: isotopes_2