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Forsmark site investigation

Hydrochemical logging of KFM04A

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March 2004

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

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Summary

Hydrochemical logging has been performed in the borehole KFM04A. Hydrochemical logging or so called tube sampling is a fast and simple sampling technique to obtain information on the chemical composition of the water column along an open borehole. The equipment consists of an approximately 1000-m long polyamide tube divided into units of 50 m length.

In most cases the water content of one tube unit constituted one sample and each second tube unit/sample was analysed. Three samples (in the beginning, in the middle and at the end of the tube array) were concatenated from two tube units in order to allow analyses of all SKB class 3 isotope options. The content of flushing water remaining in the borehole after drilling was acceptable (below 25%) in the first 300 m and the SKB class 3 isotopes will be determined in the first three samples. Beneath 300 m, the flushing water content showed a steady increase and ended at 53% in the last sample from 895–995 m. Accordingly, the isotope analyses were omitted in these samples. The relative charge balance error did not exceed the acceptable limit of $\pm 5\%$ in any of the nine samples.

Due to the high content of remaining flushing water, the analysis data obtained from the activity will be less useful for chemical modelling work.

Sammanfattning

Hydrokemisk loggning har utförts i borrhålet KFM04A. Hydrokemisk loggning eller så kallad slangprovtagning är en snabb och enkel provtagningsteknik för att få information om den kemiska sammansättningen av vattenpelaren längs ett öppet borrhål. Utrustningen består av en ungefär 1000 m lång slang, uppdelad på 50 m långa slang-enheter.

I de flesta fall utgjorde vattnet i en slangenhet ett prov och var annan slangenhet/prov analyserades. Tre prov (i början, i mitten och i slutet av slanggraden) bestod av vattenvolymen från två slangenheter. Detta för att ge tillräcklig volym för analys av samtliga isotoptillval enligt SKB klass 3. Halten kvarvarande spolvatten i borrhålet efter borrnings var acceptabel (under 25 %) i de första 300 m och SKB klass 3 isotoper kommer att analyseras i de tre första proven. Under 300 m, visade spollvattenhalten en stadig ökning och slutade vid 53 % i det sista provet från 895–995 m. Isotopanalyserna fick därför utgå för dessa prov. Det relativa jonbalansfelet överskred inte godkännande-gränsen på $\pm 5\%$ i något av de nio proven.

På grund av den höga spollvattenhalten är de analysdata som erhållits från aktiviteten inte fullt ut användbara för hydrokemisk modellering.

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1 Introduction

This document reports performance of and results from the activity “Hydrochemical logging in KFM04A” performed within the site investigation at Forsmark /1/. The work was conducted according to the Activity Plan AP PF 400-03-99 (SKB internal controlling document).

Borehole KFM04A is the fourth deep telescopic borehole drilled at the site investigations in the Forsmark area /2/. The location of the borehole and the drilling site DS4 within the investigation area is shown in Figure 1-1, whereas Figure 1-2 displays a zooming in towards drilling site DS4 with KFM04A and nearby situated percussion drilled boreholes in rock and soil. Borehole KFM04A is inclined 60° from the horizontal plane and penetrates the altered zone at the border of the candidate area. The borehole section 0–107.4 m is percussion drilled, and at the logging occasion it was cased with a stainless steel casing with the internal diameter 200 mm, whereas section 107.4–1001.42 m is core drilled with a diameter of 77 mm. 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). A borehole being of SKB chemical type entails cleaning procedures of all in-hole equipment to be used in the borehole during and after drilling according to level 2 in the cleaning instructions in MD 600.004 (Instruction for cleaning borehole equipment and certain surface equipment). The Method Descriptions and Instructions mentioned are SKB internal controlling documents. Basic borehole information is given in Table 1-1 below and the design of the borehole is presented in Appendix 1.

Table 1-1. Borehole information, KFM04A at drilling site DS4.

| Activities performed | Date of completion | Length (m) | Comment |
|---|--------------------|----------------|---|
| Percussion drilling | 2003-05-27 | 0–107.42 | – |
| BIPS-logging | 2003-06-02 | 0–106.5 | – |
| Core drilling | 2003-11-19 | 107.42–1001.42 | HFM10 served as source of flushing water for drilling the cored part of KFM04A. HFM10 is a SKB chemical type of borehole. The flushing water volume used was 655 m ³ . |
| Mammoth pumping during/ after core drilling | – | – | Pumped volume: 3466 m ³ . |
| BIPS logging | 2003-12-06 | 108–1000 | – |
| Radar logging | 2003-12-07 | 100–998 | – |
| Hydrochemical logging | 2003-12-08 | 100–1000 | Described in this report. |

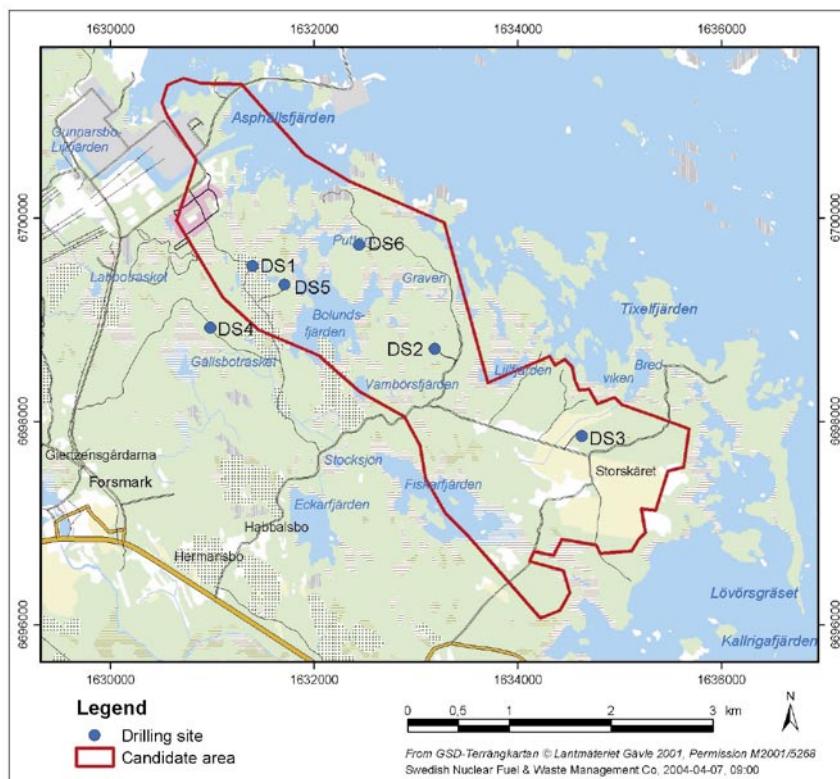


Figure 1-1. The investigation area at Forsmark (approximately the area inside the black square) including the candidate area selected for more detailed investigations. The six drilling sites for deep boreholes, DS1-6 are marked with blue circles. Borehole KFM04A is situated at drilling site DS4. Map design: Helena Nyman.

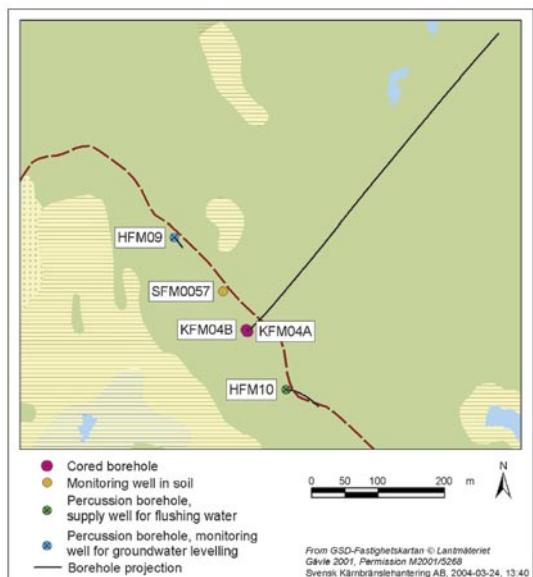


Figure 1-2. Locations of the telescopic borehole KFM04A (inclined 60°) as well as percussion boreholes and a shallow monitoring well at drilling site DS4. Map design: Helena Nyman.

2 Objective and scope

Hydrochemical logging is performed in order to obtain an overview of the initial chemical composition of the water column along the open borehole KFM04A. The sampling technique is fast and simple even at great depth.

The analysis program is carried out according to SKB chemistry class 3 including isotope options. However, if the content of drilling water in a sample exceeds 25%, the isotope determinations are omitted.

3 Sampling equipment

The sampling equipment used for the hydrochemical logging consists of an approximately 1000-m long polyamide tube divided into units of 50 m length. The equipment is described in the method description SKB MD 422.001 (Metodbeskrivning för hydrokemisk loggning, SKB internal controlling document).

A schematic illustration of the equipment used for hydrochemical logging is shown in Figure 3-1. The tube units are connected with metal couplings. The length of each tube unit is given in Table 3-1. The external and internal diameters of the tube units are 10 and 8 mm respectively. The water content in each tube unit will constitute 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 it stretched in the borehole. At both ends of each tube unit there is a manual shut off valve.

Table 3-1. Length of tube units.

| Unit | Length [m] |
|---------------------------|----------------|
| 1 | 49.71 |
| 2 | 50.08 |
| 3 | 49.77 |
| 4 | 49.28 |
| 5 | 49.97 |
| 6 | 50.01 |
| 7 | 49.85 |
| 8 | 49.87 |
| 9 | 49.57 |
| 10 | 49.72 |
| 11 | 49.67 |
| 12 | 50.25 |
| 13 | 50.62 |
| 14 | 49.70 |
| 15 | 49.22 |
| 16 | 49.20 |
| 17 | 49.30 |
| 18 | 49.63 |
| 19 | 49.62 |
| 20 | 49.87 |
| Sum: | 994.91 |
| Coupling length: | 2.812 |
| Weight length | 0.817 |
| Total tube length: | 998.539 |

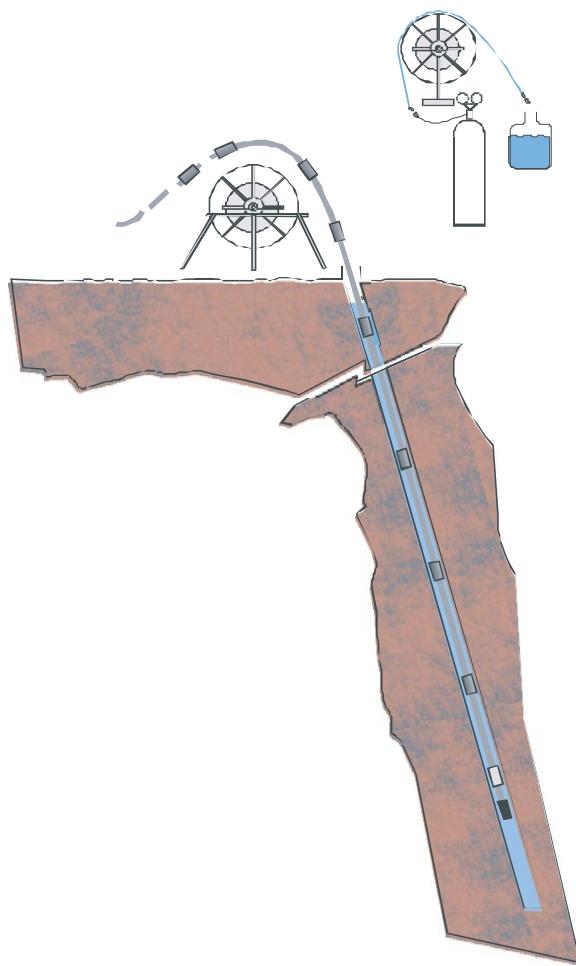


Figure 3-1. Equipment for hydrochemical logging in boreholes. At the lower end of the tube array there is a check valve and a weight connected. Each tube unit is approximately 50 m long.

4 Performance

4.1 Hydrochemical logging

Sampling of the telescopic borehole KFM04A was performed according to activity plan AP PF 400-03-99 (SKB internal controlling document) following the method described in SKB MD 422.001 (Metodbeskrivning för hydrokemisk loggning).

The hydrochemical logging was performed on the 8:th of December to a borehole length of 995 m. The tube array was not lowered all the way down to the bottom at 1001.42 m in order to decrease the risk of getting stuck and also to avoid suspending drilling debris sedimented at the bottom of the borehole. The lowering of the tubes started at 09:12 and the retrieval of the tube units started at 13:50. The first tube unit at the top of the array was lowered to 45 m of its length. Since the ground water table was situated about 7 m below top of casing, altogether about 12 m of the upper tube unit was not water filled. 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, SKB samples number 8171, 8177 and 8185 were concatenated from two tube units in order to allow analyses of all SKB class 3 isotope options.

The exact level of the ground water table in the borehole prior to logging was 7.04 m below top of casing.

4.2 Sample treatment and chemical analyses

An overview of sample treatment and analysis routines is given in Appendix 2. The routines are applicable independent of sampling method or sampling object. An overview showing the filled sample portions at the logging occasion is given in Table 4-1. The samples SKB no 8175 to 8185 were collected but not sent to the laboratories for isotope analyses due to their high content of flushing water remaining from drilling (more than 25%). The data from the hydrochemical logging are stored in the database SICADA in field note no Forsmark 243. The SKB sample numbers are 8169–8185.

Table 4-1. Overview of samples collected at hydrochemical logging in KFM04A. Filled cells represent collected samples.

| Sample information | | | Collected sample portions | | | | | | | | | | | |
|--------------------|------------|---------|---------------------------|-------------|------|--------|---------|----------------|--|------------------------|------------------|-----------|-----------------------|-------------|
| Tube unit | Length [m] | SKB no. | Cond., pH, alk. | Major comp. | Br/I | Anions | Uranine | ³ H | $\delta^{2\text{H}}/\delta^{18\text{O}}$ | $\delta^{37}\text{Cl}$ | ⁸⁷ Sr | C isotope | $\delta^{34}\text{S}$ | Left overs* |
| 1 | 0 45 | 8169 | | | | | | | | | | | | |
| 2 | 95 | 8170 | | | | | | | | | | | | |
| 3&4 | 195 | 8171 | | | | | | | | | | | | |
| 5 | 245 | 8172 | | | | | | | | | | | | |
| 6 | 295 | 8173 | | | | | | | | | | | | |
| 7 | 345 | 8174 | | | | | | | | | | | | |
| 8 | 395 | 8175 | | | | | | x | x | x | x | x | | |
| 9 | 445 | 8176 | | | | | | | | | | | | |
| 10&11 | 545 | 8177 | | | | | | x | x | x | x | x | x | |
| 12 | 595 | 8178 | | | | | | | | | | | | |
| 13 | 645 | 8179 | | | | | x | x | x | x | x | x | | |
| 14 | 695 | 8180 | | | | | | | | | | | | |
| 15 | 745 | 8181 | | | | | x | x | x | x | x | x | | |
| 16 | 795 | 8182 | | | | | | | | | | | | |
| 17 | 845 | 8183 | | | | | x | x | x | x | x | x | | |
| 18 | 895 | 8184 | | | | | | | | | | | | |
| 19&20 | 995 | 8185 | | | | | x | x | x | x | x | x | x | |

Even sample numbers are archive samples, i.e. dark grey cells.

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

4.3 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 $\pm 10\%$).

$$\text{Rel. Error (\%)} = 100 \times \frac{(\sum \text{cations(equivalents)} - \sum \text{anions(equivalents)})}{(\sum \text{cations(equivalents)} + \sum \text{anions(equivalents)})}$$

- 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 4-1.

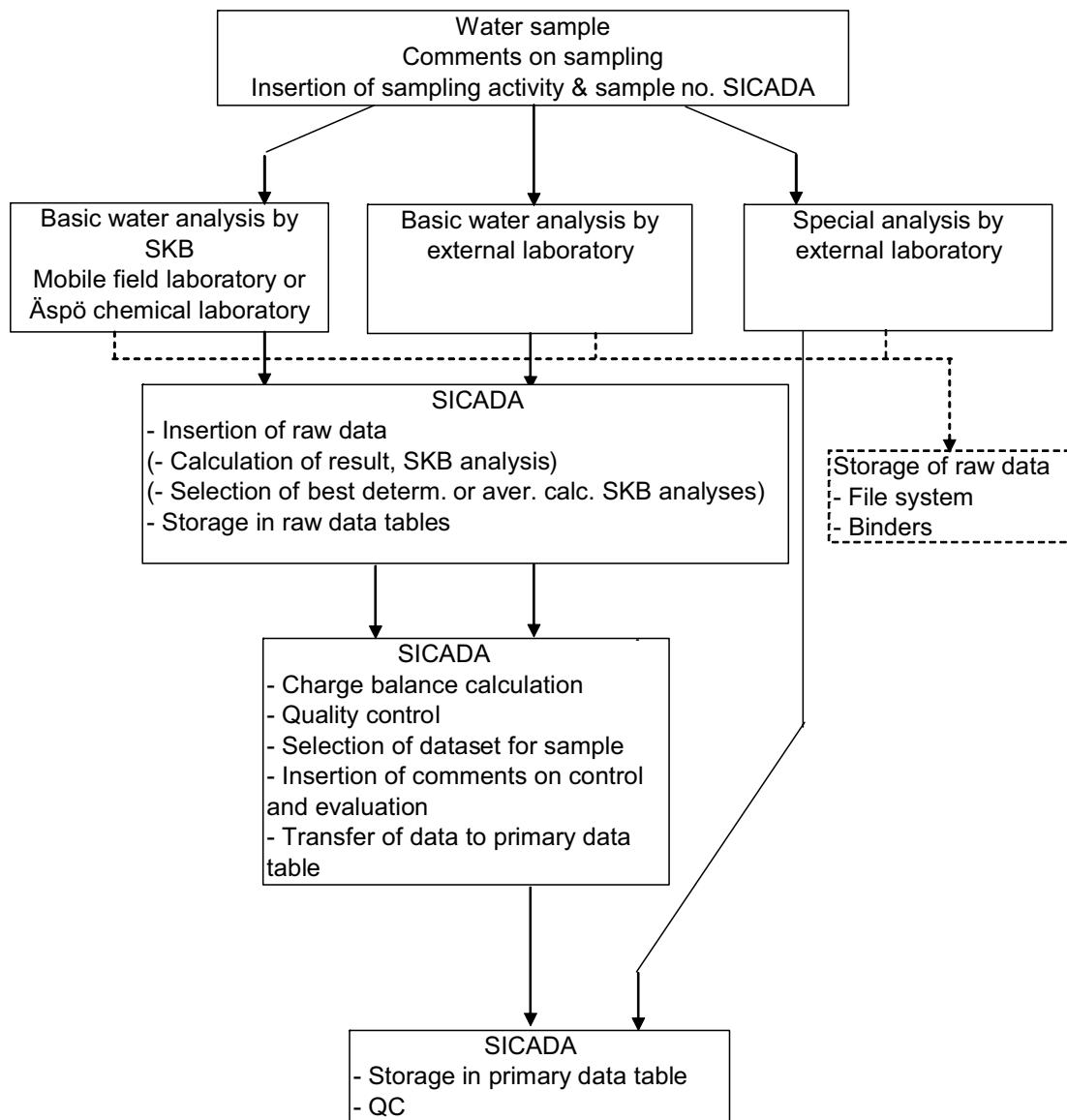


Figure 4-1. Overview of data management for hydrogeochemical data.

4.4 Nonconformities

The activity was performed according to the Activity Plan AP PF 400-03-99 and the Method Description SKB MD 422.001 without any deviations that can affect the quality of the data.

5 Results

5.1 Analysis results

The analysis data from the hydrochemical logging in borehole KFM04A are presented in Appendix 3 and 4. Diagrams showing the flushing water content and the electric conductivity plotted versus borehole length are presented in Figure 5-1 and 5-2 below. The results have been plotted for the mid-point of each tube unit, for example tube number 1 from borehole length 0–45 m is plotted at 22.5 m and so on. Isotope results are not available from 300 m and downwards to the bottom of the borehole as the flushing water content in these samples exceeded the acceptable level of 25%, see Figure 5-1.

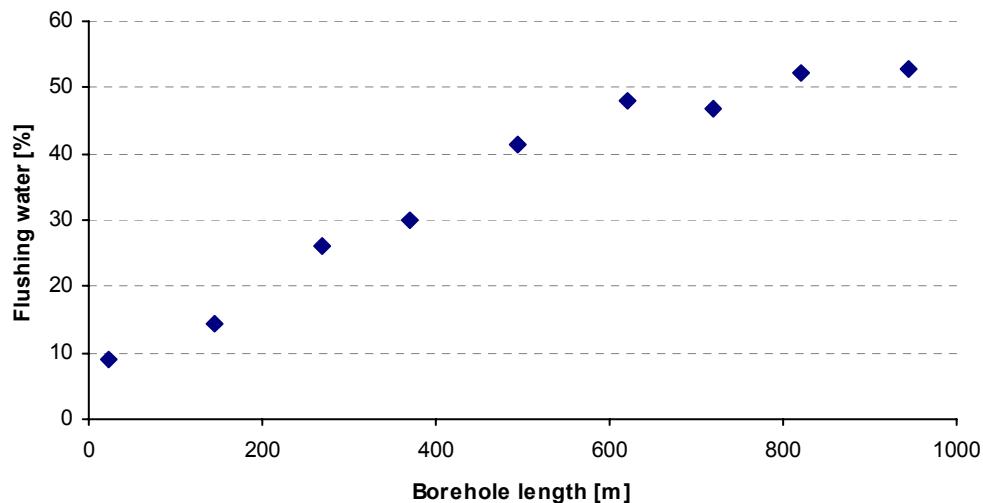


Figure 5-1. Flushing water content versus borehole length.

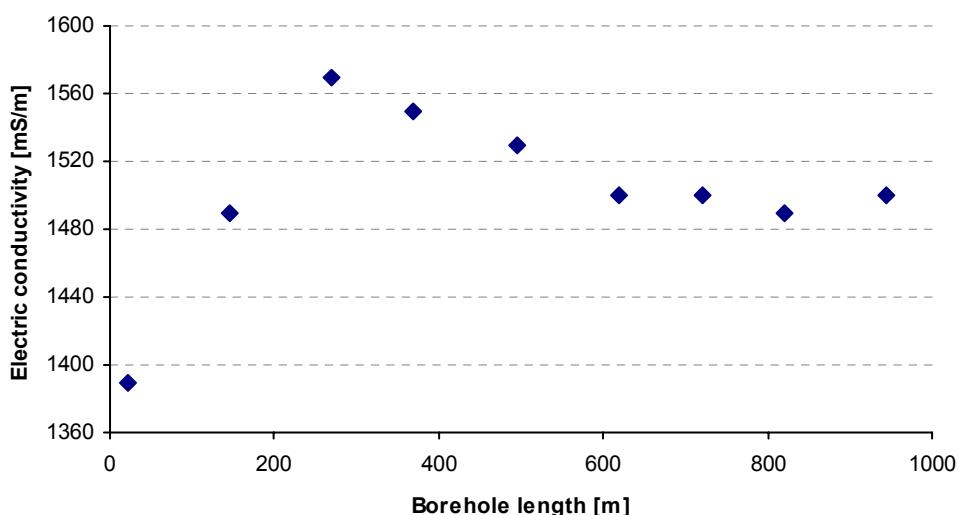


Figure 5-2. Electric conductivity versus borehole length.

5.2 Quality of the analyses

The relative charge balance errors give an indication of the quality and uncertainty of the analyses of the major components. The calculated relative charge balance errors for the selected sets of data do not in any case exceed the acceptable level of $\pm 5\%$, see Appendix 3.

6 Conclusions

The hydrochemical logging in KFM04A revealed the high content of flushing water in the water column along the open borehole. Accordingly, the analysis data obtained, will be less useful for chemical modelling work due to this fact. The main conclusions that can be drawn from the activity are:

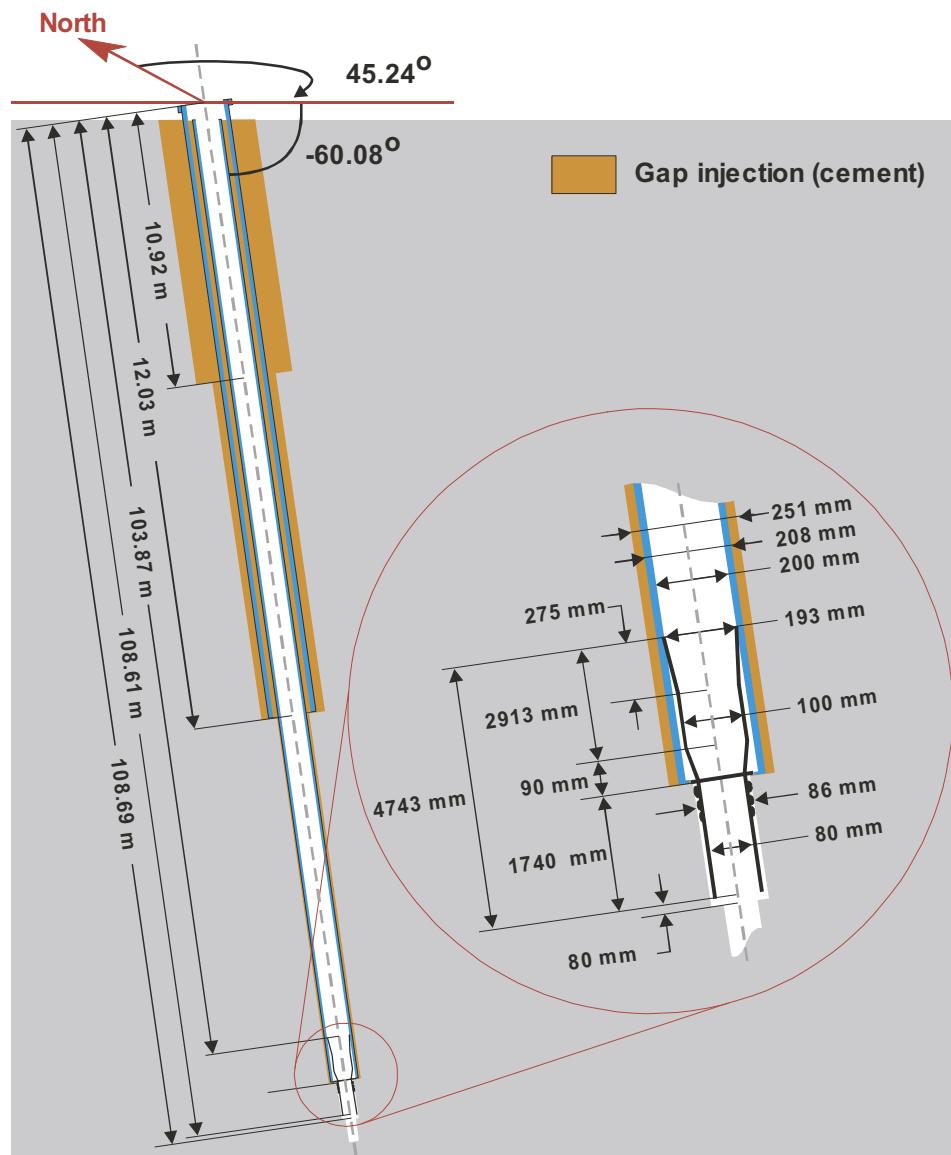
- The content of flushing water remaining in the borehole after drilling was acceptable in the first 300 m and due to this, class 3 isotope options were included for the first three samples. Beneath 300 m, the flushing water content showed a steady increase and ended at 53% in the last sample from 895–995 m.
- The relative charge balance error did not exceed the acceptable limit of $\pm 5\%$ in any case.
- At the sampling occasion, the difference flow logging was not performed yet. The electric conductivity and the flushing water content along the borehole indicate that the water yielding fractures are located in the upper part of the borehole (down to approx. 300 or 400 m).
- In order to obtain representative samples during the chemical characterisation activity, it may be necessary to conduct extra “clean up” pumping in the borehole prior to sampling.

7 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, 2003.** Forsmark site investigation. Drilling of the telescopic borehole KFM04A at drilling site DS4 (in progress), Svensk Kärnbränslehantering AB

Design of the telescopic borehole KFM04A

Technical data Borehole KFM04A



Drilling reference point

Northing: 6698921.74 (m), RT90 2,5 gon V 0:-15
 Easting: 1630978.96 (m), RT90 2,5 gon V 0:-15
 Elevation: 8.77 (m), RHB70

Drilling period

Drilling start date: 2003-05-20
 Drilling stop date: 2003-11-19

Borehole

Lenght: 1001.42 m

Appendix 2

Sampling and analysis methods

Table A2-1. Sample handling routines and analysis methods.

| Component group | Component/element | Sample container (material) | Volume (mL) | Filtering | Preparation/Conservation* | Analysis method | Laboratory*** | 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 | Mobile field lab. AnalyCen | 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) | Äspö:s chemistry lab. AnalyCen | Not critical (month) |
| | Br, I | Plastic | 100 | Yes (not in the field) | No | ICP MS | Paavo Ristola OY Analytica AB, | 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 | Analytica AB, AhalyCen | 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 | Analytica AB, AhalyCen | Not critical (month) |
| Fe(II), Fe(tot) | Fe(II), Fe(tot) | Plastic (Acid washed) | 500 | Yes | Yes (5 mL HCl) | Spectrophotometry Ferrozine method | Mobile field lab. AhalyCen 1 Äspö:s chemistry lab. | As soon as possible the same day |
| Hydrogen sulphide | HS ⁻ | Glass (Winkler) 120x2 | About | No | Ev 1 mL 1 M NaOH + 1 mL 1M ZnAc | Spectrophotometry | AhalyCen 1 Äspö:s chemistry lab. AhalyCen 1 | Immediately or if conserved, a few days |
| Nutrient salts | NO ₂ , NO ₃ ⁺ ,NO ₂ , NH ₄ , PO ₄ ³⁻ | Plastic | 250 | No | No | Spectrophotometry | Äspö:s chemistry lab. AhalyCen 1 | 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 | Analytica AB, AnalyCen | Not critical (month) |
| Lanthanoids, 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 | SGAB Analytica, AnalyCen | Not critical (month) |

| Component group | Component/ element | Sample container (material) | Volume (mL) | Filtering | Preparation/ Conservation* | Analysis method | Laboratory*** | 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 | Paavo Ristola OY Dept. of System ecology, SU | Short transportation time |
| Total organic Carbon | TOC | Plastic | 250 25 | No | Frozen, transported in isolated bag | UV oxidation, IR Carbon analysator Shimadzu TOC5000 | Paavo Ristola OY Dept. of System ecology, SU | Short transportation time |
| Environmental isotopes | $\partial^{2}H$, $\partial^{18}O$ | Plastic | 100 | No | - | MS | IFE | Not critical (month) |
| Tritium, Chlorine-37 | ^{3}H (enhanced.) $\partial^{37}Cl$ | Plastic (dry bottle) Plastic | 500 100 | No No | - | LSC ICP MS | Univ. of Waterloo | Not critical (month) |
| Carbon isotopes | $\partial^{13}C$, pmC (^{14}C) | Glass (brown) | 100×2 | No | - | (A)MS | Univ. of Waterloo | A few days |
| Sulphur isotopes | $\partial^{34}S$ | Plastic | 500–1000 | Yes | - | Combustion, ICP MS | IFE | No limit |
| Strontium-isotopes | ^{87}Sr / ^{86}Sr | Plastic | 100 | Yes | - | TIMS | IFE | Days or Week |
| Uranium and Thorium isotopes | ^{234}U , ^{235}U , ^{238}U , ^{222}Th , ^{230}Th | Plastic | 50 | Nej | - | Chemical separat. Alfa/gamma spectrometry | IFE | No limit |
| Boron isotopes | ^{10}B / ^{11}B | Plastic | 100 | Yes | Yes (1 mL HNO_3) | ICP – MS | Analytica AB | No limit |
| Radium and Radium isotopes | ^{222}Rn , ^{226}Ra | Plastic | 500 | No | No | EDA, RD-200 | IFE | 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 | Paavo Ristola OY | 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 | Analytica AB | Immediate transport |
| Humic and fulvic acids | Fractionation | Fractions are collected in plastic bottles | 250 | - | N_2 atmosphere | UV oxidation, IR (DOC) | Paavo Ristola OY | 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 | Laboratory*** | Analysis within - or delivery time to lab. |
|---|---|------------------------------------|--------------------|------------------|-----------------------------------|------------------------|----------------------------------|---|
| Carbon isotopes in humic and fulvic acids | $\partial^{13}\text{C}$, pmC (^{14}C) | DEAE cellulose (anion exchanger) | - | - | - | (A)MS | The Ångström Laboratory, Uppsala | A few days |

* Suprapur acid is used for conservation of samples.

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

*** Full name and address is given in Table A2-3.

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 A2-2. 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 | mg/L | 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 | mg/L | 15 % | |
| F ⁻ | IC | 0.2 | 0.6 | mg/L | 10 % | 20 % |
| F ⁻ | Potentiometri | - | - | mg/L | - | - |
| 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 uncertainties² | "Total" uncertainties³ |
|---------------------------------|---------------|------------------------|---------------------------------|-------------------------------|--|--|
| $\delta^{34}\text{S}$ | ICP MS | - | 0.2 ‰ | ‰ CDT ⁹ | 0.2 ‰ | - |
| $^{87}\text{Sr}/^{86}\text{Sr}$ | MS | - | - | No unit (ratio) ¹⁰ | 0.000020 | - |
| $^{10}\text{B}/^{11}\text{B}$ | ICP MS | - | - | No unit (ratio) ¹⁰ | 0,0020 | - |

- 1. Reporting limits at salinity $\leq 0.4\%$ (520 mS/m) and $\leq 3.5\%$ (3810 mS/m) respectively.
 - 2. Measurement uncertainty reported by consulted laboratory.
 - 3. Estimated total uncertainty by experience (includes effects of sampling and sample handling).
 - 4. Per mill deviation¹¹ from SMOW (Standard Mean Oceanic Water).
 - 5. TU=Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of 10^{-18} (1 Bq/L Tritium = 8.45 TU).
 - 6. Per mill deviation¹¹ from SMOC (Standard Mean Oceanic Chloride).
 - 7. Per mill deviation¹¹ from PDB (the standard PeeDee Belemnite).
 - 8. 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.
 - 9. Per mill deviation¹¹ from CDT (the standard Canyon Diablo Troilite).
 - 10. Isotope ratio without unit.
 - 11. Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:
- $$\delta^y I = 1000 \times (K_{\text{sample}} - K_{\text{standard}}) / K_{\text{standard}}$$
, where K= the isotope ratio and $^yI = ^2\text{H}, ^{18}\text{O}, ^{37}\text{Cl}, ^{13}\text{C}$ or ^{34}S etc.

Table A2-3. Participant laboratories

| |
|---|
| Äspö water chemical laboratory (SKB) Mobile field laboratory, Forsmark (SKB) |
| Inainööritoimisto Paavo Ristola Oy Teollisuus-ja Voimalaitoskemia Rajantorpartie 8, C-talo 01600 Vantaa FINLAND |
| Dept. of System ecology Stockholm University 10691 Stockholm |
| Analytica AB Aurorum 10 977 75 Luleå (Nytorpsvägen 16 Box 511 183 25 Täby) |
| Environmental Isotope Laboratory Dep. of earth sciences University of Waterloo Waterloo, Ontario N2L 3G1 CANADA |
| Institutt for energiteknik (IFE) Insituttveien 18 P.O Box 40 2027 Kjeller NORGE |
| AlnalyCen Nordic AB Box 905 531 19 Lidköping |
| The Ångström laboratory Box 534 Se-751 21 Uppsala |

Appendix 3

Water composition, compilation of basic water analysis data

| Idcode | Setup m | Seclow m | Sample no. | Date | Time | Charge Bal % | Na mg/L | K mg/L | Ca mg/L | Mg mg/L | HCO ₃ ⁻ mg/L | Cl ⁻ mg/L | SO ₄ ²⁻ mg/L | SO ₄ -S mg/L | Br mg/L | F ⁻ mg/L | Si mg/L | Li mg/L | Sr mg/L | pH | ElCond mS/m | Water % | T mg/L |
|--------|------------|-------------|---------------|------------|-------------|-----------------|------------|-----------|------------|------------|---------------------------------------|-------------------------|---------------------------------------|----------------------------|------------|------------------------|------------|------------|------------|------|----------------|------------|-----------|
| KFM04A | 0 | 45 | 8169 | 2003-12-08 | 09:12-13:50 | -2,6 | 1570 | 20,4 | 1070 | 192 | 148 | 4690 | 449 | 144 | 18,1 | 2,00 | 6,5 | 0,049 | 11,6 | 7,20 | 1390 | 9,09 | 0,041 |
| KFM04A | 45 | 95 | 8170 | 2003-12-08 | 09:12-13:50 | -2,5 | 1680 | 21,9 | 1170 | 204 | 124 | 5080 | 477 | 151 | 19,3 | 0,65 | 6,2 | 0,050 | 12,5 | 7,17 | 1490 | xxx | - |
| KFM04A | 95 | 195 | 8171 | 2003-12-08 | 09:12-13:50 | -2,4 | 1780 | 23,5 | 1250 | 211 | 95 | 5410 | 501 | 156 | 21,2 | <0,2 | 5,3 | 0,053 | 13,5 | 6,98 | 1570 | xxx | - |
| KFM04A | 195 | 245 | 8172 | 2003-12-08 | 09:12-13:50 | -2,4 | 1785 | 23,2 | 1240 | 208 | 82 | 5410 | 493 | 155 | 21,1 | <0,2 | 5,1 | 0,053 | 13,7 | 6,87 | 1550 | xxx | - |
| KFM04A | 245 | 295 | 8173 | 2003-12-08 | 09:12-13:50 | -2,5 | 1780 | 23,2 | 1240 | 208 | 82 | 5410 | 493 | 155 | 21,1 | <0,2 | 5,1 | 0,053 | 13,7 | 6,87 | 1550 | xxx | - |
| KFM04A | 295 | 345 | 8174 | 2003-12-08 | 09:12-13:50 | -2,5 | 1785 | 23,2 | 1240 | 208 | 82 | 5410 | 493 | 155 | 21,1 | <0,2 | 5,1 | 0,053 | 13,7 | 6,87 | 1550 | xxx | - |
| KFM04A | 345 | 395 | 8175 | 2003-12-08 | 09:12-13:50 | -2,5 | 1780 | 23,2 | 1240 | 208 | 82 | 5410 | 493 | 155 | 21,1 | <0,2 | 5,1 | 0,053 | 13,7 | 6,87 | 1550 | xxx | - |
| KFM04A | 395 | 445 | 8176 | 2003-12-08 | 09:12-13:50 | -2,3 | 1750 | 23,1 | 1230 | 198 | 70 | 5300 | 490 | 151 | 21,3 | <0,2 | 4,5 | 0,052 | 13,7 | 6,76 | 1530 | xxx | - |
| KFM04A | 445 | 545 | 8177 | 2003-12-08 | 09:12-13:50 | -2,3 | 1750 | 23,1 | 1230 | 198 | 70 | 5300 | 490 | 151 | 21,3 | <0,2 | 4,5 | 0,052 | 13,7 | 6,76 | 1530 | xxx | - |
| KFM04A | 545 | 595 | 8178 | 2003-12-08 | 09:12-13:50 | -2,4 | 1720 | 23,0 | 1200 | 193 | 59 | 5200 | 478 | 148 | 21,2 | 0,4 | 4,2 | 0,051 | 13,5 | 6,69 | 1500 | 47,9 | 0,046 |
| KFM04A | 595 | 645 | 8179 | 2003-12-08 | 09:12-13:50 | -2,4 | 1720 | 23,0 | 1200 | 193 | 59 | 5200 | 478 | 148 | 21,2 | 0,4 | 4,2 | 0,051 | 13,5 | 6,69 | 1500 | xxx | - |
| KFM04A | 645 | 695 | 8180 | 2003-12-08 | 09:12-13:50 | -2,1 | 1720 | 23,2 | 1200 | 192 | 55 | 5180 | 473 | 147 | 20,3 | <0,2 | 4,1 | 0,051 | 13,5 | 6,59 | 1500 | 46,8 | 0,044 |
| KFM04A | 695 | 745 | 8181 | 2003-12-08 | 09:12-13:50 | -2,7 | 1710 | 23,3 | 1190 | 191 | 53 | 5210 | 471 | 145 | 20,9 | <0,2 | 4,2 | 0,051 | 13,4 | 6,52 | 1490 | 52,2 | 0,045 |
| KFM04A | 745 | 795 | 8182 | 2003-12-08 | 09:12-13:50 | -2,0 | 1710 | 23,8 | 1210 | 191 | 51 | 5170 | 472 | 145 | 20,6 | <0,2 | 4,5 | 0,051 | 13,5 | 6,50 | 1500 | xxx | - |
| KFM04A | 795 | 845 | 8184 | 2003-12-08 | 09:12-13:50 | -2,0 | 1710 | 23,8 | 1210 | 191 | 51 | 5170 | 472 | 145 | 20,6 | <0,2 | 4,5 | 0,051 | 13,5 | 6,50 | 1500 | 52,7 | 0,046 |
| KFM04A | 845 | 895 | 8185 | 2003-12-08 | 09:12-13:50 | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | - | |

- = Archive sample
xxx = not collected
< "value" = result less than detection limit

ChargeBal % = Relative charge balance error %
SICADA: water_composition, 040225

Appendix 4

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

| ldcode | Secup | Seclow | Sample | Date | Time | $\delta^2\text{H}$ | $\delta^3\text{H}$ | $\delta^{18}\text{O}$ | $\delta^{34}\text{S}$ | $\delta^{37}\text{Cl}$ | $\delta^{13}\text{C}$ | $^{87}\text{Sr}/^{86}\text{Sr}$ | ^{14}C |
|--------|-------|--------|--------|------------|-------------|--------------------|--------------------|-----------------------|-----------------------|------------------------|-----------------------|---------------------------------|-----------------|
| m | m | no | | | | dev SMOW | TU | dev SMOW | dev CDT | dev SMOC | dev PDB | no unit | pmC |
| KFM04A | 0 | 45 | 8169 | 2003-12-08 | 09:12-13:50 | -74,3 | A | -9,30 | — | A | — | — | — |
| KFM04A | 95 | 195 | 8171 | 2003-12-08 | 09:12-13:50 | -73,7 | A | -9,20 | — | A | — | — | — |
| KFM04A | 245 | 295 | 8173 | 2003-12-08 | 09:12-13:50 | -70,9 | A | -9,00 | — | A | — | — | — |

- = Not analysed
 A = results will be reported later
 x = No result due to sampling problems
 xx = No result due to analytical problems
 SiCADA: h_o_isotopes, b_s_cl_sr_isotopes, c_s_isotopes 040405