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Forsmark site investigation

Hydrochemical monitoring of percussion- and core drilled boreholes

Results from water sampling and analyses during 2005

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April 2006

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Keywords: Forsmark, AP PF 400-05-060, Long-term monitoring, Percussion borehole, Core borehole, Groundwater, Water sampling, Chemical analyses, Isotopes, Uranium, Colloids, Fractionation, Filtration.

Abstract

The first year of groundwater sampling within the long-term hydrogeochemical monitoring programme for percussion drilled and core drilled boreholes is completed and is documented in the present report. The programme includes sampling twice a year in boreholes with installed equipment for long-term pressure monitoring, for tracer tests and for water sampling in packed off borehole sections. The first year comprised sampling of groundwater in eight borehole sections corresponding to seven boreholes at the first sampling occasion and two more sections in an additional borehole at the next occasion. The number of boreholes in the programme will increase the next few years as more boreholes will be equipped with the necessary installations.

Besides the main objective, to obtain long time series of chemical data, the monitoring programme gives a good opportunity to investigate chemical issues arisen from earlier investigations. Due to the high uranium concentrations that were observed at inter-mediate depths in boreholes KFM02A and KFM03A, a complementary uranium study was initiated. Such high concentrations should be difficult to dissolve at reducing conditions. The first step, to investigate if uranium is present as colloids in the ground-water, was taken during 2005. The next step during 2006 will be to determine the oxidation state of the uranium.

The results constituted groundwater chemistry data in accordance with SKB chemistry class 3 including the isotopes ^{3}H, δ^{18}O and δD (first sampling) as well as SKB chemistry class 5 (second sampling). The results suggest that only a few borehole sections show significant changes in the chloride concentration compared to earlier investigations. Furthermore, uranium colloid data from different fractionation/filtration experiments were obtained together with corresponding data for other major elements, trace elements and DOC (Dissolved Organic Carbon). The uranium study in KFM02A and KFM03A indicated that a minor part of the uranium is present as a fraction > 1,000 D (1 Dahlton = 1 g/mol) in the groundwaters. This part is, however, far too small to provide a final explanation of the high uranium concentrations.

Sammanfattning

Första årets grundvattenprovtagning inom det hydrokemiska programmet för långtidsövervakning av hammarborrhål och kärnborrhål är slutförd och dokumenteras i denna rapport. Programmet innefattar provtagning två gånger om året i borrhål med installerad utrustning för långtidsövervakning av tryck, för spårförsök och för vattenprovtagning i avmanschetterade borrhålssektioner. Första året omfattade provtagning i åtta borrhålssektioner och sju borrhål vid första provtagningstillfället och ytterligare två sektioner i ett tillkommande borrhål vid nästa tillfälle. Antalet borrhål kommer att öka under de kommande åren vartefter fler borrhål förses med de nödvändiga installationerna.

Förutom det huvudsakliga syftet, att erhålla långa tidsserier av kemidata, ger moniteringsprogrammet goda möjligheter att undersöka kemiska frågeställningar som uppstått vid tidigare undersökningar. På grund av de höga urankoncentrationerna som observerades i djupintervallet vid cirka 400–600 m i KFM02A och KFM03A, initierades en kompletterande uranundersökning. Så höga halter borde vara svåra att få i lösning under reducerande förhållanden. Första steget, att undersöka om uranet förekommer som kolloidfas i grundvattnet, genomfördes under 2005. Nästa steg, under 2006, kommer att innebära undersökning av uranets oxidationstal.

Resultaten består av grundvattenkemiska data enligt SKB:s kemiklass 3 med isotop-tillvalen ^{3}H, δ^{18}O och δD (första provtagningstillfället) och SKB:s kemiklass 5 (andra provtagningstillfället). Av resultaten framgår att endast några borrhålssektioner uppvisar signifikanta skillnader i kloridhalt jämfört med tidigare undersökningar. Vidare erhölls urandata för kolloider vid olika fraktionerings/filtreringsförsök tillsammans med motsvarande data för andra huvudelement och spårelement samt DOC (Dissolved Organic Carbon). Uranstudien i KFM02A och KFM03A indikerar att endast en mindre andel av uranet föreligger som en kolloidfraktion > 1,000 D (1 Dahlton = 1 g/mol) i grundvattnen. Denna andel är emellertid alltför liten för att ge en fullständig förklaring till de höga urankoncentrationerna.

Contents

1 Introduction

This document reports the performance of and the results from the first year of the hydrogeochemical monitoring program for percussion drilled and core drilled boreholes. The sampling programme is one of the activities performed within the site investigation at Forsmark and the work was carried out in accordance with activity plan AP PF 400-05-060. The controlling documents for performing this activity are listed in Table 1-1. Both activity plan and method descriptions are SKB's internal controlling documents. The field work was performed in June and November 2005. The obtained data are reported in the SICADA database and are traceable by the activity plan number.

The hydrogeochemical monitoring activity performed during 2005 included water sampling and chemical analyses in the boreholes and borehole sections listed in Table 1-2.

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

Activity plan	Number	Version
Hydrokemiskt övervakningsprogram för hammarborrhål och kärnborrhål under 2005.	AP PF 400-05-060	1.0
Measurement system descriptions	**Number**	**Version**
Mätsystembeskrivning (MSB) – Handhavande del; System för hydrologisk och metrologisk datainsamling. Vattenprovtagning och utspädningsmätning i observationshål.	SKB MD 368.010	1.0
Mätsystembeskrivning (MSB) – Handhavande del; Fraktionering av humus- och fulvosyror med membranfiltrering.	SKB MD 431.043	1.0

Table 1-2. Boreholes, borehole sections and section transmissivities included in the monitoring programme for percussion- and core drilled boreholes during 2005.

Borehole: section	Section borehole length [m]	Transmissivity [m^2/s]
KFM01A:5	109.0–130.0	8.6 E–8*
KFM02A:3	490.0–518.0	2.1 E–6*
KFM02A:5	411.0–442.0	2.5 E–6*
KFM03A:1	969.5–994.5	5.5 E–7*
KFM03A:4	633.5–650.0	2.4 E–6*
HFM02:2	38.0–48.0	5.9 E–4**
HFM04:2	58.0–66.0	7.9 E–5**
HFM13:1	159.0–173.0	2.9 E–4**
HFM15:1	85.0–95.0	1.0 E–4**
HFM19:1	168.0–182.0	2.7 E–4**

* From injection tests /P-04-95, P-04-100, P-04-194, P-05-145/.
** From flow loggings /P-03-33, P-03-34, P-04-71, P-04-72/.

KFM01A, KFM02A and KFM03A are former SKB chemistry-type, subvertical, and approximately 1,000 m long, telescopic boreholes, whereas HFM02, HFM04, HFM13, HFM15 and HFM19 are percussion boreholes with lengths varying between 99.5 to 221.7 m. Technical descriptions and designs of the boreholes are presented in P-03-30, P-03-32, P-03-51, P-03-52, P-03-59, P-04-85 and P-04-106 and the installations for long-term monitoring of pressures and chemical compositions are described in PIR-04-13/14/27 and PIR-05-17/18/20/23/24 (all PIR reports are SKB internal documents). The site investigation area in Forsmark as well as the locations of the monitored boreholes are shown in Figure 1-1.

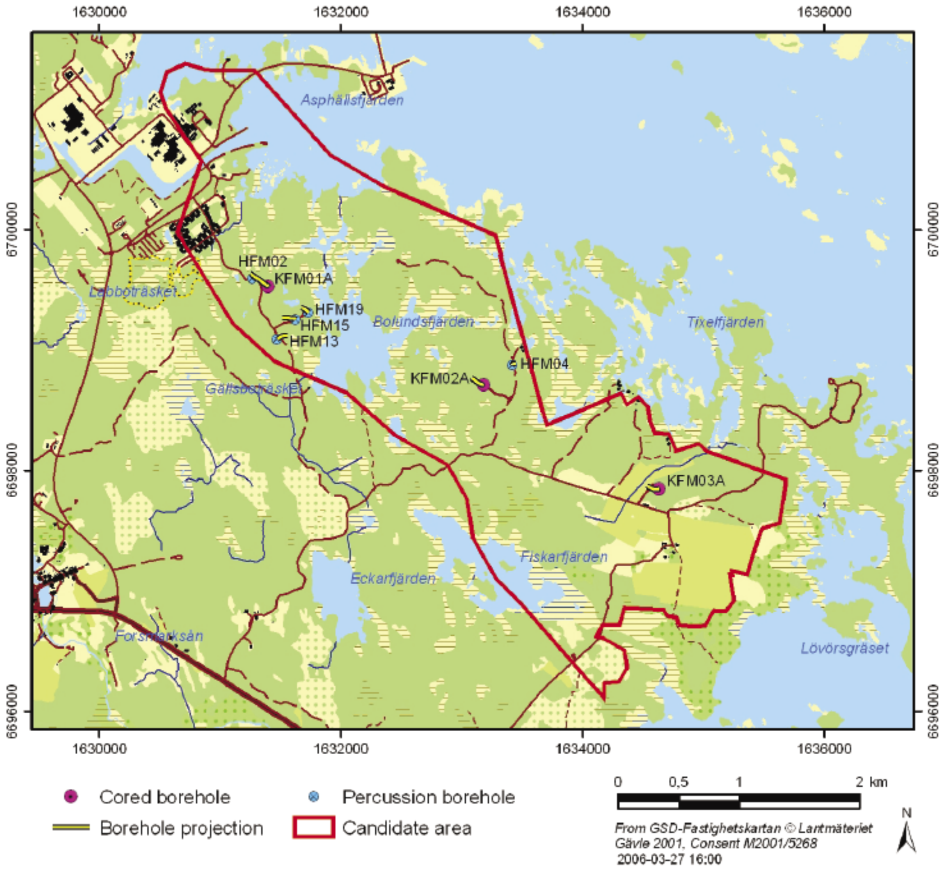

Figure 1-1. *General overview over the Forsmark site investigation area. Sampled boreholes within the monitoring program 2005 are marked with blue (percussion) and pink (telescopic) infilled circles.*

2 Objective and scope

The long-term hydrogeochemical monitoring programme for percussion drilled and core drilled boreholes aims at creating long time series of data. The main objective is to observe possible changes in the water composition for example due to that the initial conditions might have been disturbed from drilling. The monitoring will also allow identification of eventual perturbation effects from other ongoing investigations. Due to the extremely high uranium concentrations that have been observed at intermediate depths in boreholes KFM02A and KFM03A /P-04-70 and P-04-108/, a special uranium investigation was also initiated. Such high concentrations should be difficult to dissolve at reducing conditions. The first step during year 2005 was to investigate if the uranium is present as colloids.

The monitoring programme comprises groundwater sampling twice a year in borehole sections delimited by "permanently" installed packers. In this context "permanently" means that the equipment stays in the borehole for several years unlike other, short-term investigations where the equipment is lifted when the investigation is completed. The number of monitored boreholes will increase the next few years when new borehole installations are completed. Generally, only the so called circulation sections are sampled. These sections are also used for groundwater flow measurements.

The monitoring includes sampling and analyses according to SKB chemistry class 3 and 5 as well as field measurements of pH, electric conductivity and temperature. Besides the ordinary programme 2005, the colloid content was studied in KFM02A at 411.0–442.0 m and 490.0–518.0 m and in KFM03A at 633.5–650.0 m, using fractionation and technique (SKB MD 431.043) and filtration through 0.05 µm filters. The focus was on uranium but also other major and trace cations and dissolved organic carbon (DOC) were analysed in the different fractions.

3 Equipment

3.1 Sampling equipment

The monitored boreholes are equipped with packer installations in order to isolate different borehole sections. Each section is connected to HMS which is a system for pressure monitoring. Outlines of the instrumentation in percussion drilled and telescopic boreholes, respectively, are presented in Figure 3-1.

Five identical pump equipments (GEOPUMP UV45) were used to retrieve the water samples from the sampled sections. An outline of the sampling setup is presented in Figure 3-2. The water passes through a coarse filter to eliminate large particles that may be present in the water, then through the mini-packer isolating the section and thereafter through the downhole pump on the way to the surface. The flow rate is controlled by varying the speed of the downhole pump with a voltage regulator at the surface.

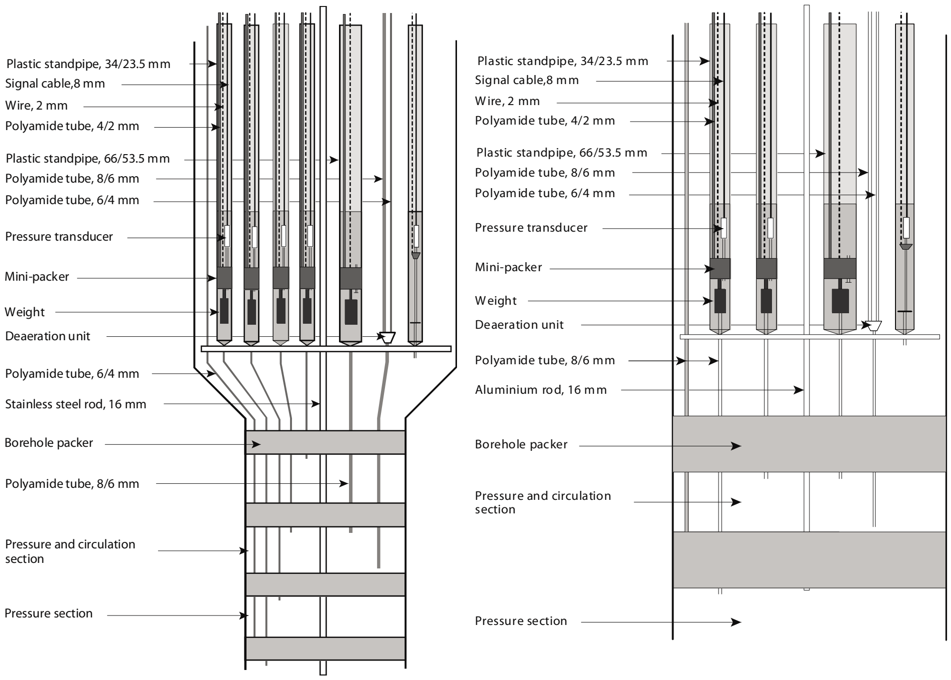

***Figure 3-1.** Instrumentation in core boreholes (left) and percussion boreholes (right) including circulation sections.*

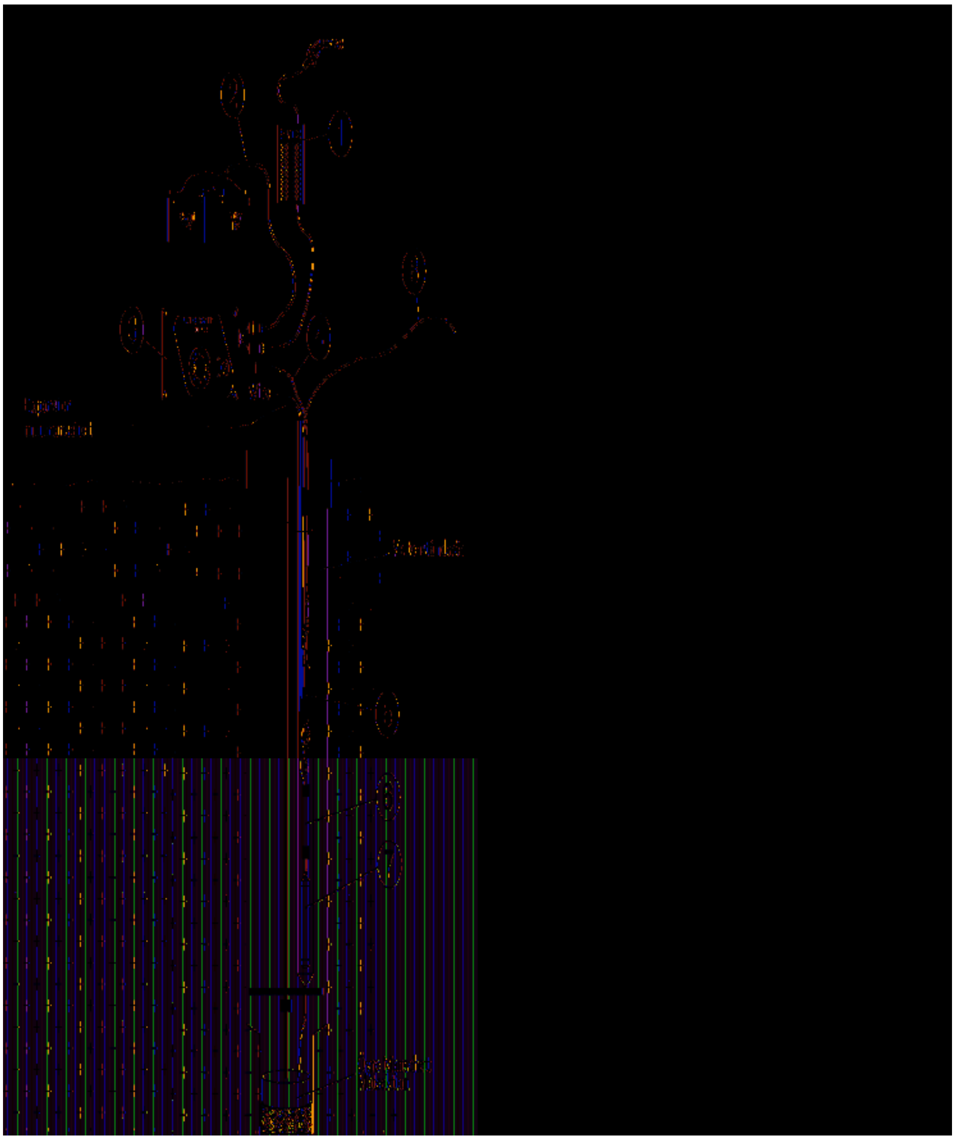

Figure 3-2. *Equipment setup used for sampling of water from circulation sections in monitored percussion drilled and telescopic boreholes. 1) voltage regulator (24 VDC), 2) battery cable (not used), 3) pump regulator, 4) pump cable, 5) pump (GEOPUMP UV 45), 6) small inflatable packer (PU 45), 7) filter (SF 45), 8) 8/6 mm polyamide tube to pump.*

3.2 Equipment used for the uranium study

The equipment for fractionation consisted of membrane filters with a defined cut-off (pore size), a membrane pump, flexible tubing and vessels. Generally, two portions of the water sample are filtered through filters with pore sizes 1,000 D and 5,000 D, respectively (D = Dalton, 1D = 1 g/mol). However, only the 1,000 D filter was used in the present study.

Figure 3-3 shows the equipment setup and Figure 3-4 illustrates the path for the water through the filter during fractionation. Furthermore, filtrations using ordinary polycarbonate filters with pore size 0.05 µm (Nucleopore polycarbonate filters) were performed. Besides the uranium species, size distributions of other inorganic and organic constituents were investigated.

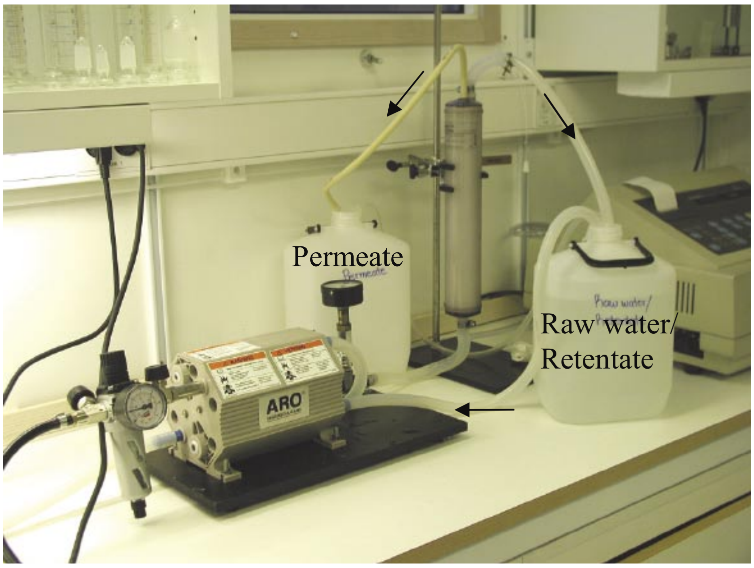

Figure 3-3. *Equipment for fractionation of humic and fulvic acids and inorganic colloids.*

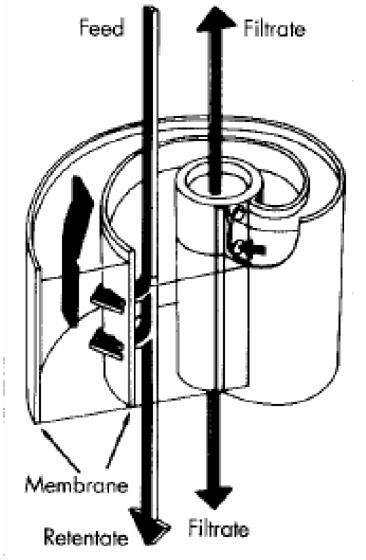

Figure 3-4. *The black arrows show the water flow through the membrane filter during filtration/fractionation.*

4 Performance

4.1 General

Monitored boreholes and borehole sections, sampling dates, collected samples and analyses performed are presented in Table 4-1.

Table 4-1. Boreholes, borehole sections, sampling dates, collected samples and analyses performed.

Idcode	Section [m]	Sampling no. 1 Date	Sample no.	Analayses	Sampling no. 2 Date	Sample no.	Analayses
HFM02	38.0–48.0	05-06-10	8915	Class 3, Tr, ^{2}H, ^{18}O	05-11-09	12006	Class 5, options
HFM04	58.0–66.0	05-06-29	8929	Class 3, Tr, ^{2}H, ^{18}O	05-11-07	12003	Class 5, options
HFM13	159.0–173.0	05-06-09	8916	Class 3+Tr, ^{2}H, ^{18}O	05-11-09	12009	Class 5, options
HFM15	85.0–95.0	06-06-09	8917	Class 3+Tr, ^{2}H, ^{18}O	05-11-09	12007	Class 5, options
HFM19	168.0–182.0	05-06-09	8914	Class 3+Tr, ^{2}H, ^{18}O	05-11-09	12010	Class 5, options
KFM01A	109.0–130.0	05-06-09	8913	Class 3+Tr, ^{2}H, ^{18}O	05-11-09	12008	Class 5, options
KFM02A	411.0–442.0	–		–	05-11-07	12002	Class 5,options*
KFM02A	490.0–518.0	–		–	05-11-07	12004	Class 5,options*
KFM03A	633.5–650.5	05-06-23	8926	Class 5+options*	05-11-07	12001	Class 5, options
KFM03A	969.5–994.5	05-06-23	8927	Class 3+Tr, ^{2}H, ^{18}O	05-11-07	12005	Class 5, options

*Including uranium study (fractionation/filtration).

4.2 Water sampling and field measurements

Prior to sampling, the water volume in each section was exchanged at least three times to obtain a representative water sample from the section. The total pumped volumes from each section prior to sampling are given in Appendix 1.

In addition to sampling of ground water, field measurements of temperature, electric conductivity and pH were conducted. Prior to collecting a sample, the water from the borehole was led through a measurement cell in which the electrodes and the thermometer were placed to measure field pH (pH_F), field electric conductivity (EC_F) and groundwater temperature, Figure 4-1. The results from the field measurements are presented in Appendix 3.

Sample portions intended for analysis of major constituents and trace metals (by ICP technique), DOC and iron (by spectrometry) were filtered on-line. Disposable 0.40 µm filters were fitted directly to the 6/8 mm polyamide-tube leading the pumped water from the borehole section. During the entire sampling, laboratory gloves were used to minimize the risk of contaminating the samples.

Figure 4-1. *Water from the borehole is lead through a measurement cell (consisting of three plastic bottles) to perform field measurements of pH, temperature and conductivity.*

4.3 The uranium study; fractionations and filtrations

This study was primarily conducted in order to investigate eventual presence of colloidal uranium which might explain the high uranium concentrations in the groundwaters at intermediate depths in KFM02A and KFM03A. However, analyses of other inorganic constituents as well as humic and fulvic acids were also performed. The investigated sections were 411.0–442.0 m and 490.0–518.0 m in KFM02A and section 633.0–650.0 m in KFM03A. Two methods were applied; 1) fractionation using ultra-filtration technique and 2) filtration through ordinary polycarbonate filters with pore size 0.05 µm.

The fractionation procedure was as follows; the water samples (5L) were first filtered on-line through normal 0.40 µm polycarbonate filters and then through a special membrane filter with a cut off size of 1,000 D. The resulting retentate and permeate volumes following the filtration runs were approximately one and four litres, respectively, giving an enrichment factor of five in the retentate.

Water samples collected from 1) the retentate and 2) the permeate as well as filtrates from 3) the 0.40 µm and 4) the 0.05 µm filters together with 5) a non-filtered sample were analysed for major constituents and uranium. Retentates, permeates and filtrates from the 0.40 µm filters were also analysed for other trace metals and dissolved organic carbon (DOC).

4.4 Water sample treatment and analyses

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.

5 Nonconformities

- At the first sampling occasion, online field measurements of electrical conductivity (EC) were performed in only three out of eight sections. Online EC values are therefore missing from KFM01A, HFM02, HFM13, HFM15 and HFM19.
- Pumping in section KFM03A:1 during the sampling in June caused pressure changes in section KFM03A:2 in the same borehole. A probable explanation is water leakage in couplings between the sections. It is impossible to estimate the effect of the leakage on the water composition in the collected sample from section KFM03A:1.
- At the second sampling occasion the pH-meter was out of function. Therefore online field measurements of pH are available only from section 633.5–650.0 m in KFM03A.
- At the second sampling occasion, drowned mice were found in HFM04 and HFM13 when lifting the packers in order to install the sampling equipment. This may have caused contamination of the collected water samples.
- Between the first and second sampling occasion, ground flow measurements and tracer tests (AP PF 400-05-037) were performed in the monitored sections. In HFM15 the fluorescent dye tracer Rhodamine WT from Holiday Dyes Inc. (techn. quality) was used in high concentration. Since the colour is very similar to the colour created in order to analyse iron by spectrophotometry (after adding reagent), this may have affected the iron analyses (Fe_{tot} and FeII). In KFM01A high concentrations of Uranine (Sodium Flourescein, from Merck, purum quality) was added 2005-07-12. Since this tracer was also used to mark the flushing water, the flushing water content cannot be determined in water samples collected after that date. Approximately 180–190 g of Rhodamine WT and 20 g of Uranine were added to HFM15 and KFM01A, respectively, during the tracer tests.

6 Data handling and interpretation

6.1 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 ± 5% are considered acceptable.

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

- 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 6-1.

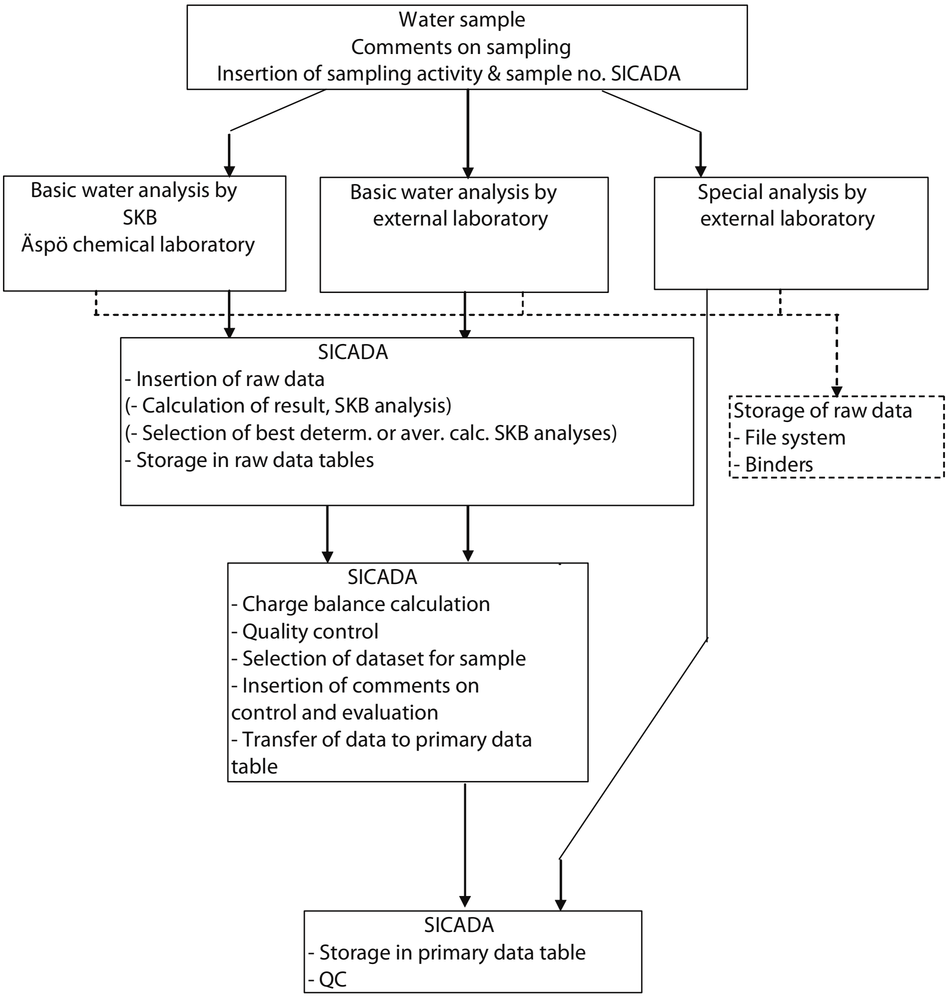

Figure 6-1. *Overview of data management for hydrogeochemical data.*

6.2 Fractionation of inorganic colloids and humic and fulvic acids

The concentrations of organic and inorganic constituents in the retentate and permeate are re-calculated to concentration values for each one of the two fractions, i.e. species with molecular weights lower or higher than the cut-off size of the filter. This is done using mass balance equations as described in SKB MD 431.043, SKB internal controlling document (cf Table 1-1).

7 Results

7.1 Water analysis

7.1.1 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, both laboratory data and field measurement data on pH and electrical conductivity (EC) were obtained and the water temperature was recorded in the field.

For samples collected in core drilled telescopic boreholes, the flushing water content is an important parameter, see Figure 7-1 (data from the previously performed chemical characterisations in the corresponding sections /P-03-94, P-04-70, P-04-108/ are presented for comparison). However, in borehole KFM01A groundwater flow measurements and tracer tests were performed in the period between the two sampling occasions and additional Uranine was used. Therefore, the only relevant flushing water content from this borehole is the one obtained from the first sampling in June. This value is also very high, most probably due to inflow of flushing water used for core drilling of the nearby situated borehole KFM01B (drilling period 2003-07-29 to 2004-01-15) /P-04-302/.

The charge balance errors provide an indication of the quality and uncertainty of the analyses of major constituents. The errors did not exceed the acceptable limit of ± 5% in any of the cases. One sample at each sampling occasion was analysed by a second laboratory. Generally, the difference in concentrations between laboratories/methods for each analysed constituent is less than 10% except for low concentrations close to the detection limits. The basic water analysis data and relative charge balance errors are compiled in Appendix 3, Table A3-1.

Chloride concentrations are presented in Figure 7-2 together with earlier results from chemical characterisations with SKB's mobile field laboratory in cored boreholes /P-03-94, P-04-70, P-04-108/ and water samplings conducted during pump test in percussion boreholes /P-03-47, P-03-48, P-04-92/.

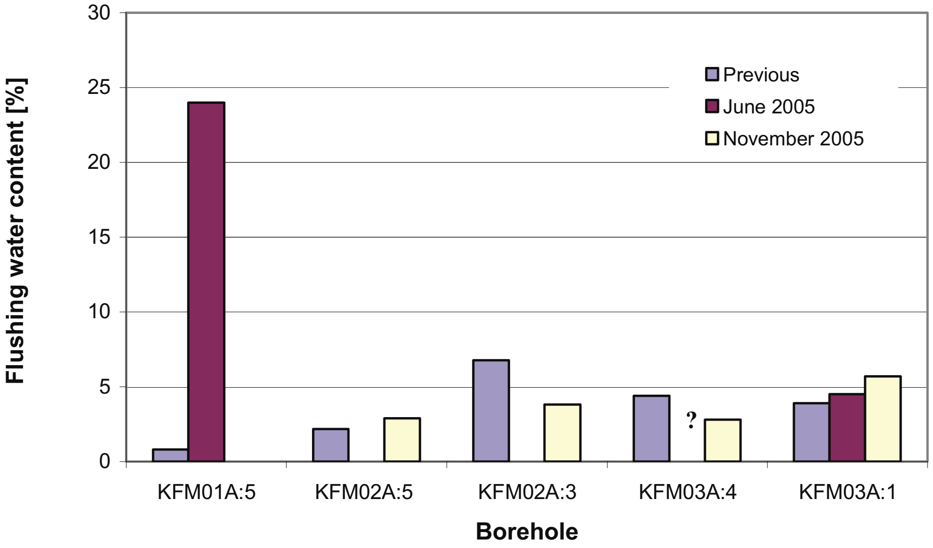

__Figure 7-1.__ Amounts of flushing water in the water samples from boreholes KFM01A, KFM02A (two borehole sections) and KFM03A (two sections). The contents at previous chemical investigations (chemical characterisations) in corresponding borehole sections are given for comparison.

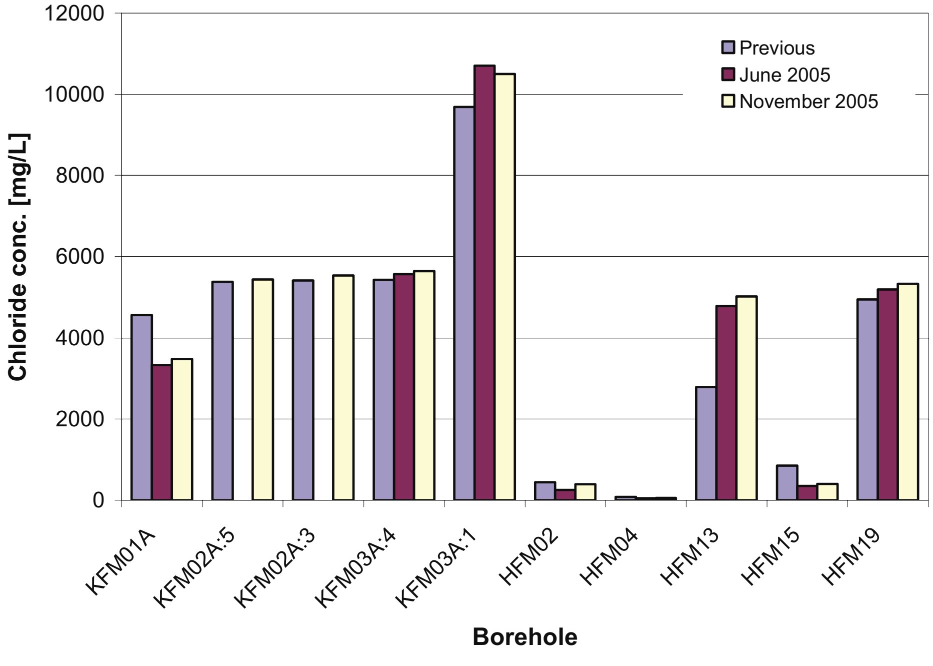

__Figure 7-2.__ Chloride concentrations in samples collected within the monitoring program. Results from earlier chemical investigations (chemical characterisations in KFM-boreholes and water sampling during pumping tests in HFM-boreholes are given for comparison. For the HFM-boreholes the initial and the present concentrations are not quite comparable as the early sampling was performed at open hole conditions from the entire borehole and not from packed off sections.

7.1.2 Trace elements (rare earth metals and others)

The sample collected in section 633.5–650.0 m in KFM03A as well as all samples collected in November were analysed for trace elements. The analyses of trace elements include U, Th, As, Sc, Cd, Hg, V, Rb, Y, Zr, In, Cs, Ba, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb as well as Lu and are compiled in Appendix 3, Table A3-2.

7.1.3 Stable and radioactive isotopes

The isotope determinations include the stable isotopes δD, δ^{18}O, ^{10}B/^{11}B, δ^{34}S, δ^{13}C and ^{87}Sr/^{86}Sr as well as the radioactive isotopes ^{3}H (TU), ^{14}C (pmC), ^{238}U, ^{234}U, ^{230}Th, ^{226}Ra and ^{222}Rn. All samples were analysed for δD, δ^{18}O and ^{3}H. The other isotopes were determined only for SKB class 5 samples. Available isotope data at the time of reporting are compiled in Appendix 3, Table A3-3 and A3-4.

A comparison between re-calculated uranium isotope determinations and ICP-analyses are given in Table 7-1. The isotope ^{238}U is converted to element concentrations using the expressions given in Appendix 2. Generally, results within the same order of magnitude indicate a satisfactory agreement.

Table 7-1. Comparison of isotope determinations of ^{238}U and ICP-analyses of the element uranium.

Borehole: Section	Sample no.	Date [yyyy-mm-dd]	^{238}U [mBq/L]	U [µg/L]	U* [µg/L]
KFM02A:3	12004	2006-11-07	1,478	122	119
KFM02A:5	12002	2006-11-07	319	25.9	25.7
KFM03A:4	8926	2005-06-23	490	46.3	39.5
KFM03A:4	12001	2005-11-09	530	45.2	42.7

* Recalculated from ^{238}U [mBq/L].
A = Analysis results to be reported.

7.2 Colloid fractions of uranium and other trace metals

The presence of uranium colloids was investigated in groundwaters from KFM02A and KFM03A by fractionation/ultra filtration using a cylindrical filter with a cut-off of 1,000 D and also by filtration through ordinary polycarbonate filters.

The uranium results constitute fractions < 1,000 D and > 1,000 D as well as uranium concentrations in filtrates through 0.4 µm and 0.05 µm filters and in unfiltered samples, see Table 7-2 and Figure 7-3. From the results it can be concluded that a minor part of the uranium is present as a size fraction with a molecular weight larger than 1,000 D. This fraction is, however, much too small to explain the high uranium concentrations observed in the waters. The uranium concentrations in the filtered and unfiltered samples agree within the error of the analysis and no detectable amount of uranium particles/colloids seems to be caught in these filters.

Besides uranium, Ca, Fe, K Mg, Na, S, Si, Al, Ba, Cd, Co, Cr, Cu, Hg, Li, Mn, Mo, Ni, Pb, Sr, V and Zn were determined in the samples from the fractionation experiments.

Table 7-2. Summary of results from the uranium study.

Section/ Fraction	KFM03A 633.5–650.0 m U [µg/L]	KFM02A 411.0–442.0 m U [µg/L]	KFM02A 490.0–518.0 m U [µg/L]
< 1,000 D	37.6 ± 6.0	23.3 ± 4.0	106 ± 18
> 1,000 D	5.3 ± 2.7	2.1 ± 1.2	9.2 ± 6.1
Non filtered	45.3 ± 7.3	26.6 ± 4.3	119 ± 20
Filtrate 0.40 µm	44.8 ± 7.2	25.9 ± 4.1	122 ± 20
Filtrate 0.05 µm	42.3 ± 7.4	26.6 ± 4.3	121 ± 19

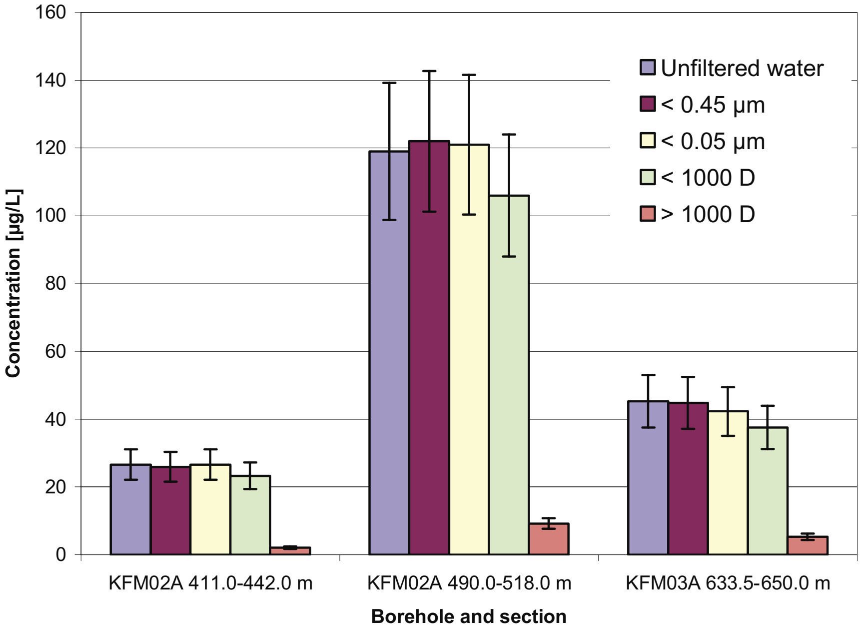

***Figure 7-3.** Uranium study in KFM02A at 411.0–442.0 m and 490.0–518.0 m and in KFM03A at 633.5–650.0 m. Uranium concentrations are presented for 1) unfiltered water, 2) filtrate through 0.40 µm filter, 3) filtrate through 0.05 µm filter, 4) fraction < 1,000 D, 5) fraction > 1,000 D.*

From these elements, only iron, silicon, sulphur, aluminium, calcium and manganese were considered important as colloid species. The aluminium results were inconsistent and impossible to interpret and are therefore rejected. The results are presented in Tables 7-3, 7-4 and 7-5 and indicate that all investigated elements except sulphur exist preferably as species with a molecular weight less than 1,000 D (g/mol). Such species are too small to be referred to as colloids. Minor colloidal fractions of sulphur have been indicated also in earlier investigations and they are not unlikely to appear. Calcite was not precipitated to any significant extent in any of the fractionation cases.

The filters were carefully washed before use and samples of de-ionised water (after passing through the washed filters) were analysed as sample blanks. The concentrations of all species except aluminium were insignificant (within the error of the analyses).

Table 7-3. Inorganic fractions in KFM02A at section 411.0–442.0 m.

Fraction	Fe [mg/L]	Si [mg/L]	S [mg/L]	Mn [µg/L]
< 1,000 D	0.99 ± 0.13	7.6 ± 1.1	135 ± 13.5	1,760 ± 299
> 1,000 D	–	–	4.1 ± 3.4	–
Adsorption	0.14 ± 0.20	–	–	–

– = Not found.

Table 7-4. Inorganic fractions in section 490.0–518.0 m in KFM02A.

Fraction	Fe [mg/L]	Si [mg/L]	S [mg/L]	Mn [µg/L]
< 1,000 D	1.31 ± 0.17	5.8 ± 0.9	148 ± 14.8	2,010 ± 342
> 1,000 D	–	–	6.3 ± 4.5	–
Adsorption	0.58 ± 0.31	–	–	–

– = Not found.

Table 7-5. Inorganic fractions in section 633.5–650.0 m in KFM03A.

Fraction	Fe [mg/L]	Si [mg/L]	S [mg/L]	Mn [µg/L]
< 1,000 D	0.84 ± 0.15	7.4 ± 1.1	77.2 ± 7.7	525 ± 89
> 1,000 D	–	–	–	–
Adsorption	0.12 ± 0.22	–	–	–

– = Not found.

7.3 Organic fractions

In addition to ICP-analysis the samples from the fractionations were also analysed for organic constituents, DOC. The results from fractionation of organic acids are summarised in Table 7-6.

As shown, the water in the two sections in KFM02A contain a small fraction of organic acids with a molecular weight larger than 1,000 D. This fraction was not detected in the groundwater of KFM03A at 633.5–650.0 m. This indicates that most of the organic constituents are present as fulvic acids and possibly other low molecular weight organic acids such as citric acid and oxalic acid. The results are consistent with previous fractionation experiments performed in these boreholes /P-04-70, P-04-108/.

Table 7-6. Summary of fractionation results in KFM02A and KFM03A.

Section/ Fraction	KFM02A 411.0–442.0 m DOC [mg/L]	KFM02A 490.0–518.0 m DOC [mg/L]	KFM03A 633.5–650.0 m DOC [mg/L]
< 1,000 D	1.0 ± 0.1	1.2 ± 0.2	1.4 ± 0.2
> 1,000 D	0.2 ± 0.05	0.3 ± 0.1	–
Adsorption	–	–	–

– = Not found.

8 Summary and discussions

The first year of groundwater sampling within the long-term hydrogeochemical monitoring programme for percussion drilled and core drilled boreholes is completed and ten borehole sections in eight boreholes have been sampled (most of them at two occasions). The monitoring programme offers a good opportunity to investigate chemical issues arisen from earlier investigations as for example the high uranium concentrations that were observed at intermediate depths in boreholes KFM02A and KFM03A. The results and conclusions from the ordinary analysis programme as well as from the special uranium study are summarised below.

- Generally, the changes in flushing water content since the initial investigations in the core drilled boreholes are small. Borehole KFM01A is the only exception. The increased flushing water content in this borehole in June is most probable due to inflow of flushing water used for core drilling of the nearby situated borehole KFM01B. Further, prior to the sampling occasion in November, ground water flow measurements and tracer tests had been performed in the same borehole and after that occasion it was no longer possible to estimate the flushing water content from the Uranine concentration.
- Only minor changes in the water composition are observed in the cored boreholes since previous investigations except for the groundwaters from the fractures at 113–119 m in KFM01A and at 940 m in KFM03A. KFM01A shows a decrease in chloride concentration (from 4,500 to 3,500 mg/L since February 2003) due to flushing water intrusion, while the chloride concentration in KFM03A has increased (from 9,700 to 10,500 mg/L since December 2003). In KFM03A a so called up-coning effect was observed after drilling. This effect was caused by the heavy pumping during and after drilling and it is reasonable to believe the conditions were disrupted at the first chemical sampling in December 2003. The present results from the percussion boreholes are not quite comparable with the initial results as the later represent open borehole conditions.
- From the uranium study it can be concluded that a minor part of the uranium is present in the groundwater as a fraction > 1,000 D, but no detectable amount of uranium particles/colloids were caught in the ordinary disposable filters. Uranium containing colloid phases does not seem to be the explanation to the high uranium concentration at intermediate depths in KFM02A and KFM03A.
- The fractionation results for organic constituents are consistent with earlier results. The sections in KFM02A reveal a minor fraction > 1,000 D but this fraction is not present in KFM03A.

References

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/P-03-32/ **Claesson L-Å, Nilsson G, 2004.** Forsmark site investigation. Drilling of the telescopic borehole KFM01A at drilling site DS1.

/P-03-33/ **Ludvigson J-E, Jönsson S, Levén J, 2003.** Forsmark site investigation. Pumping tests and flow logging. Boreholes KFM01A (0–100 m), HFM01, HFM02 and HFM03.

/P-03-34/ **Ludvigson J-E, Jönsson S, Svensson T, 2003.** Forsmark site investigation. Pumping tests and flow logging. Boreholes KFM02A (0–100 m), HFM04 and HFM05.

/P-03-47/ **Nilsson A-C, 2003.** Forsmark site investigation. Sampling and analyses of groundwater in percussion drilled boreholes and shallow monitoring wells at drillsite DS1. Results from the percussion boreholes HFM01, HFM02, HFM03, KFM01A (borehole section 0–100 m) and the monitoring wells SFM0001, SFM0002 and SFM0003.

/P-03-48/ **Nilsson A-C, 2003.** Forsmark site investigation. Sampling and analyses of groundwater in percussion drilled boreholes and shallow monitoring wells at drillsite DS2. Results from the percussion boreholes HFM04, HFM05, KFM02A (borehole section 0–100 m) and the monitoring wells SFM0004 and SFM0005.

/P-03-51/ **Claesson L-Å, Nilsson G, 2003.** Forsmark site investigation. Drilling of a flushing water well, HFM05, and a groundwater monitoring well, HFM04 at HFM03, at drillsite DS2.

/P-03-52/ **Claesson L-Å, Nilsson G, 2004.** Forsmark site investigation. Drilling of the telescopic borehole KFM02A at drilling site DS2.

/P-03-59/ **Claesson L-Å, Nilsson G, 2004.** Forsmark site investigation. Drilling of the telescopic borehole KFM03A and the core drilled borehole KFM03B at drilling site DS3.

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/P-04-85/ **Claesson L-Å and Nilsson G, 2004.** Forsmark site investigation. Drilling of a flushing water well, HFM13, two groundwater monitoring wells in solid bedrock, HFM14-15, and one groundwater monitoring well in soil, SFM0058, at and close to drilling site DS5.

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/P-04-302/ **Claesson L-Å and Nilsson G, 2005.** Forsmark site investigation. Drilling of the borehole KFM01B at drilling site DS1.

/P-04-108/ **Wacker P, Bergelin A, Berg C and Nilsson A-C, 2004.** Forsmark site investigation. Hydrochemical characterisation in KFM03A. Results from six investigated borehole sections: 386.0–391.0 m, 448.0–453.0 m, 448.5–455.6 m, 639.0–646.1 m, 939.5–946.6 m, 980.0–1,001.2 m.

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/P-05-145/ **Svensson T, Ludvigson J-E and Hjerne C, 2005.** Forsmark site investigation. Single-hole injection tests in borehole KFM02A, re-measurements after hydraulic fracturing.

Appendix 1

Sampling information and field measurements

Idcode: section	Pumping Start	Stop	Pumped volume [dm³]	Sampling Date	Start	Stop	Field measurements Date	Start	Stop	Sample no.
HFM02:2	2005-06-08 14:40	2005-06-10 09:20	724	2005-06-10	9:15	9:20	2005-06-10	9:05	9:15	8915
HFM02:2	2005-11-08 16:19	2005-11-09 08:12	333	2005-11-09	7:35	8:11	2005-09-11	7:30	7:35	12006
HFM04:2	2005-06-28 11:30	2005-06-29 13:45	788	2005-06-29	13:35	13:40	2005-06-29	13:25	13:35	8929
HFM04:2	2005-11-04 13:12	2005-11-07 13:53	392	2005-11-07	13:30	13:53	2005-11-07	13:27	13:30	12003
HFM13:1	2005-06-08 15:10	2005-06-09 16:35	732	2005-06-09	16:35	16:40	2005-06-09	16:30	16:35	8916
HFM13:1	2005-11-08 15:10	2005-11-09 10:51	319	2005-11-09	10:25	10:50	2005-11-09	10:23	10:25	12009
HFM15:1	2005-06-08 14:50	2005-06-09 16:10	836	2005-06-09	16:05	16:10	2005-06-09	16:00	16:05	8917
HFM15:1	2005-11-08 15:46	2005-11-09 11:02	497	2005-11-09	10:25	10:55	2005-11-09	10:57	11:00	12007
HFM19:1	2005-06-08 15:02	2005-06-09 16:25	914	2005-06-09	16:20	16:25	2005-06-09	16:15	16:20	8914
HFM19:1	2005-11-09 10:14	2005-11-09 16:05	176	2005-11-09	15:37	16:04	2005-11-09	15:34	15:37	12010
KFM01A:5	2005-06-08 14:10	2005-06-09 15:40	122	2005-06-09	15:35	15:40	2005-06-09	15:30	15:35	8913
KFM01A:5	2005-11-08 15:05	2005-11-09 11:46	99	2005-11-09	11:15	11:45	2005-11-09	11:00	11:05	12008
KFM02A:3	2005-11-04 14:07	2005-11-07 14:45	218	2005-11-07	14:35	15:07	2005-11-07	14:33	14:35	12004
KFM02A:5	2005-11-04 14:47	2005-11-07 16:05	167	2005-11-07	14:07	14:33	2005-11-07	14:05	14:07	12002
KFM03A:1	2005-06-22 11:05	2005-06-23 13:40	798	2005-06-23	13:35	13:40	2005-06-23	13:30	13:35	8927
KFM03A:1	2005-11-04 10:12	2005-11-07 13:05	404	2005-11-07	12:40	13:05	2005-11-07	11:24	11:30	12005
KFM03A:4	2005-06-22 11:05	2005-06-23 13:59	484	2005-06-23	13:05	13:58	2005-06-23	12:55	13:05	8926
KFM03A:4	2005-11-04 10:54	2005-11-07 11:19	391	2005-11-07	10:45	11:19	2005-11-07	10:35	10:45	12001

Appendix 2

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	Yes (not in the field)	No	Titration Pot. meas, Cond. meas	The same day – maximum 24 hours
Anions 2	Cl, SO_4, Br^-, F^-, I^-	Plastic	100	Yes (not in the field)	No	Titration (Cl^-) IC (Cl^-, SO_4, Br^-, F^-) ISE (F^-)	Not critical (month)
	Br, I	Plastic	100	Yes (not in the field)	No	ICP MS	Not critical (month)
Cations, Si and S according to SKB class 3	Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr	Plastic (at low conc. acid washed bottles)	100	Yes (not in the field)	Yes (not in the field, 1 mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Cations, Si and S according to SKB class 4 and 5	Na, K, Ca, Mg, S(tot), Si(tot), Fe, Mn, Li, Sr	Plastic (Acid washed)	100	Yes (immediately in the field)	Yes (1mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic (Acid washed)	500	Yes	Yes (5 mL HCl))	Spectrophotometry Ferrozine method	As soon as possible the same day
Hydrogen sulphide	HS^-	Glass (Winkler)	About 120×2	No	Ev 1 mL 1 M NaOH+1 mL 1M ZnAc	Spectrophotometry	Immediately or if conserved, a few days
Environmental metals	Al, As, Ba, B, Cd, Co, Cr, Cu, Hg, Mo, Ni, P, Pb, V, Zn	Plastic (Acid washed)	100	Yes	Yes (1 mL HNO_3)	ICP-AES ICP-MS	Not critical (month)
Lantanoids, U, Th and so on.	Sc, Rb, Y, Zr, I, Sb, Cs, La, Hf, Tl, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, U, Th	Plastic (Acid washed)	100	Yes	Yes (1 mL HNO3)	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 analysator Shimadzu TOC5000	Short transportation time

Component group	Component/ element	Sample container (material)	Volume (mL)	Filtering	Preparation/ Conservation*	Analysis method	Analysis within – or delivery time to lab.
Total organic Carbon	TOC	Plastic	250 25	No	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time
Environmental isotopes	^{2}H, ^{18}O	Plastic	100	No	– –	MS	Not critical (month)
Tritium	^{3}H (enhanced.)	Plastic (dry bottle)	500	No	–	LSC	
Chlorine-37	Chlorine-37	Plastic	100	No	–	ICP MS	Not critical (month)
Carbon isotopes	^{13}C, ^{14}C	Plastic (HDPE)	100×2	No	–	(A)MS	A few days
Sulphur isotopes	^{34}S	Plastic	500 –1,000	No	–	Combustion, ICP MS	No limit
Strontium-isotopes	$^{87}Sr/^{86}Sr$	Plastic	100	No	–	TIMS	Days or Week
Uranium and Thorium isotopes	^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th,	Plastic	50 1,000	No	–	Chemical separat. Alfa/gamma spectrometry	No limit
Boron isotopes	^{10}B	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP – MS	No limit
Radon and Radium isotopes	^{222}Rn, ^{226}Ra	Plastic	500–1,000	No	No	EDA, RD-200	Immediate transport
Dissolved gas (content and composition)	Ar, N_2, CO_2, O_2, CH_4, H_2, CO, C_2H_2, C_2H_4, C_2H_6, C_3H_8	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series	Polycarbonate filter	0.4, 0.2 and 0.05 µm	–	Ar atmosphere	ICP-AES ICP-MS	Immediate transport
Fractionation; Humic and fulvic acids, inorganic constituents	< 1,000 D > 1,000 D but < 5,000 D > 5,000 D	Fractions are collected in plastic bottles	250	–	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	Yes (in the field)	No, frozen immediately***	Spectro-photometry	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	Elementaranalysator (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×c 120	No	Mn (II) reagent Iodide reagent	Spectrophotometry SIS SS-EN 25813	Within 3 days
Archive samples for supplementary radio nuclides		Plastic	5,000	No	50 mL HNO_3	–	Storage in freeze container

* Suprapur acid is used for conservation of samples.

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

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

Abbreviations and definitions:

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

Table 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^- Cl^-	Mohr-titration IC	> 70 1–100	mg/L	5% 6%	< 10% 10%
SO4	IC	1	mg/L	10%	15%
Br^- Br^-	IC ICP	0.2 0.001	mg/L	9% 15%	20%
F^- F^-	IC Potentiometric	0.1 –	mg/L	10% –	20%
I^-	ICP	0.001	mg/L	15%	20%
Na	ICP	0.1	mg/L	4%	10%
K	ICP	0.4	mg/L	6%	15%
Ca	ICP	0.1	mg/L	4%	10%
Mg	ICP	0.09	mg/L	4%	10%
S(tot)	ICP	0.160	mg/L	21%	15%
Si(tot)	ICP	0.03	mg/L	4%	15%
Sr	ICP	0.002	mg/L	4%	15%
Li	ICP	0.2[1] 2	mg/L	10%	20%
Fe	ICP	0.4[1] 4	mg/L	6%	10%
Mn	ICP	0.03[1] 0.1	µg/L	8%	10%
Fe(II), Fe(tot)	Spectrophotometry	0.02 (DL = 0.005 mg/L)	mg/L	15% (> 30 µg/L)	20%
HS^-	Spectrophotometry	SKB 0.03 (DL = 0.02)	mg/L	10%	30%
NO_2 as N	Spectrophotometry	0.1	µg/L	2%	20%
NO_3 as N	Spectrophotometry	0.2	µg/L	5%	20%
NO_2+NO_3 as N	Spectrophotometry	0.2	µg/L	0.2 (0.2–20 µg/L) 2% (> 20 µg/L)	20%
NH_4 as N	Spectrophotometry	0.8	µg/L	0.8 (0.8–20 µg/L) 5% (> 20 µg/L)	20%
		50 (SKB)		20%	
PO_4 as P	Spectrophotometry	0.7	µg/L	0.7 (0.7–20 µg/L) 3% (> 20 µg/L)	20%

Component	Method	Reporting limits or range		Unit	Measurement uncertainty[2]	”Total” uncertainty[3]
SiO_4	Spectrophotometry	1		µg/L	3% (> 200 µg/L)	–
O_2	Jodometrisc 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%[4]
Ba, Cr, Mo, Pb	ICP	0.01		µg/L	7–10%	20%[4]
Cd, Hg	ICP	0.002		µg/L	9 resp 5%	20%[4]
Co, V	ICP	0.005		µg/L	8 resp 5%	20%[4]
Cu	ICP	0.1		µg/L	8%	20%[4]
Ni	ICP	0.05		µg/L	8%	20%[4]
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	0.005[1]	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%
$\delta^{2}H$	MS	2		‰ SMOW[5]	1‰	–
$\delta^{18}O$	MS	0.1		‰ SMOW[5]	0.2‰	–

Component	Method	Reporting limits or range	Unit	Measurement uncertainty[2]	”Total” uncertainty[3]
^{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]	–	–
$\delta^{13}C$	A (MS)	–	‰ PDB[8]	–	–
^{14}C pmc	A (MS)	–	PMC[9]	–	–
$\delta^{34}S$	ICP MS	0.2‰	‰ CDT[10]	0.3‰	–
$^{87}Sr/^{86}Sr$	TIMS	–	No unit (ratio)[11]	–	–
$^{10}B/^{11}B$	ICP MS	–	No unit (ratio) [11]	–	–
^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{230}Th	Alfa spectr.	0.0005	Bq/L[12]	5%	–
^{222}Rn, ^{226}Rn	LSC	0.03	Bq/L	5%	–

[1] Reporting limits at salinity ≤ 0.4% (520 mS/m) and ≤ 3.5% (3810 mS/m) respectively.

[2] Measurement uncertainty reported by consulted laboratory, generally 95% confidence interval.

[3] Estimated total uncertainty by experience (includes effects of sampling and sample handling).

[4] Determined only in surface waters and near surface groundwater.

[5] Per mille deviation[13] from SMOW (Standard Mean Oceanic Water).

[6] TU = Tritium Units, where one TU corresponds to a Tritium/hydrogen ratio of 10^{-18} (1 Bq/L Tritium = 8.45 TU).

[7] Per mille deviation[13] from SMOC (Standard Mean Oceanic Chloride).

[8] Per mille deviation[13] from PDB (the standard PeeDee Belemnite).

[9] The following relation is valid between pmC (percent modern carbon) and Carbon-14 age:
$pmC = 100 \times e^{((1,950-y-1.03t)/8,274)}$ where y = the year of the C-14 measurement and t = C-14 age.

[10] Per mille deviation[13] from CDT (the standard Canyon Diablo Troilite).

[11] Isotope ratio without unit.

[12] The following expressions are applicable to convert activity to concentration, for uranium–238 and thorium–232: 1 ppm U = 12.4 Bq/kg^{238}U 1 ppm Th = 3.93 Bq/kg^{232}Th.

[13] Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:
$\delta^{y}I = 1{,}000\times(K_{sample}-K_{standard})/K_{standard}$, where K = the isotope ratio and ^{y}I = ^{2}H, ^{18}O, ^{37}Cl, ^{13}C or ^{34}S etc.

Appendix 3

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	SO4_S mg/L	Br mg/l	F^- mg/L	Si mg/L	Fe mg/L
HFM02	38.00	48.00	8915	2005-06-10	–0.82	247	12.5	53	15.5	408	255	60.4	19.9	2.47	1.68	7.05	0.214
HFM02	38.00	48.00	12006	2005-11-09	1.46	339	14	68	20.9	407	396	83.7	27.8	1.91	2.34	6.28	0.417
HFM04	58.00	66.00	8929	2005-06-23	–1.52	144	6.93	29.8	7.4	388	48.4	43.6	15.9	0.207	1.72	7.43	0.213
HFM04	58.00	66.00	12003	2005-11-07	0.36	153	6.04	31	7.6	390	56	44.8	14.2	0.234	2.21	6.83	0.348
HFM13	159.00	173.00	8916	2005-06-09	–1.50	1,590	25.4	1,160	181	129	4,780	443	160	22.3	1.21	8.36	0.952
HFM13	159.00	173.00	12009	2005-11-09	–1.05	1,710	25.2	1,180	198	124	5,020	476	160	23.7	1.33	7.73	3.11
HFM15	85.00	95.00	8917	2005-06-09	–0.62	298	9.26	107	13.6	451	354	105	39.0	2.57	1.68	8.16	1.210
HFM15	85.00	95.00	12007	2005-11-09	1.18	358	9.37	97.2	15.2	471	406	104	34.4	2.02	2.33	7.62	1.02
HFM19	168.00	182.00	8914	2005-06-09	–3.12	1,930	56.2	904	242	122	5,190	539	186	21.5	1.08	6.55	3.530
HFM19	168.00	182.00	12010	2005-11-09	–1.45	2,050	57.2	960	259	129	5,330	565	196	14.7	1.15	6.39	5.40
KFM01A	109.00	130.00	8913	2005-06-09	–2.0	1,310	19.2	650	82.8	207	3,330	135	51.2	17.3	1.24	11.0	0.123
KFM01A	109.00	130.00	12008	2005-11-09	–0.80	1,430	20.7	658	95.3	136	3,480	223	75.7	16.4	1.40	9.73	0.434
KFM02A	411.00	442.00	12002	2005-11-07	–0.11	1,930	26.3	1,240	201	96.5	5,440	435	136	26.5	1.43	7.82	1.24
KFM02A	490.00	518.00	12004	2005-11-07	–2.65	2,160	36.4	890	244	126	5,540	507	157.0	24.3	1.47	6.08	1.85
KFM03A	633.50	650.00	8926	2005-06-23	–0.24	1,820	22.1	1,530	80.4	31.5	5,570	232	92	37.1	1.33	8.07	0.896
KFM03A	633.50	650.00	12001	2005-11-09	0.11	1,850	21.6	1,550	80.2	33.7	5,640	230	77.8	40.8	1.3	7.33	0.981
KFM03A	969.50	994.50	8927	2005-06-23	–0.69	2,100	10	4,140	10.8	7.46	10,700	46.1	19.3	92.2	1.32	5.72	< 0.04
KFM03A	969.50	994.50	12005	2005-11-07	0.05	2,120	12.8	4,110	9.6	10.7	10,500	47	15.3	151.0	1.38	4.85	1.09

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pH_F; EC_F = Field measurements of pH and EC.
< "value" = below reporting limit
RCB % = Rel. charge balance error %
SICADA: water_composition

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Fe-tot mg/L	FeII mg/L	Mn mg/L	Li mg/L	I^- mg/L	pH	pH_F	DOC mg/L	TOC mg/L	HS^- mg/L	Drill-water%	ElCond mS/m	EC_F mS/m
HFM02	38.00	48.00	8915	2005-06-10	–	–	0.10	0.011	–	7.76	7.81	–	–	–	–	157	–
HFM02	38.00	48.00	12006	2005-11-09	0.438	0.431	0.127	0.014	0.01	7.82	–	9.8	9.5	0.026	–	206	216
HFM04	58.00	66.00	8929	2005-06-23	–	–	0.06	0.008	0.007	7.73	7.85	–	–	–	–	84	89.9
HFM04	58.00	66.00	12003	2005-11-07	0.353	0.351	0.0804	0.006	0.005	7.71	–	8.3	8.3	0.047	–	87.9	116.8
HFM13	159.00	173.00	8916	2005-06-09	–	–	2.06	0.072	0.044	7.27	7.33	–	–	–	–	1,410	–
HFM13	159.00	173.00	12009	2005-11-09	3.45	3.47	2.15	0.052	0.053	7.34	–	2.2	A	0.023	–	1,460	1,436
HFM15	85.00	95.00	8917	2005-06-09	–	–	0.65	0.012	–	7.32	7.33	–	–	–	–	203	–
HFM15	85.00	95.00	12007	2005-11-09	1.25	1.23	0.467	0.013	0.02	7.44	–	13.0	13.0	0.206	–	220	220
HFM19	168.00	182.00	8914	2005-06-09	–	–	1.78	0.079	< 0.04	7.07	7.24	–	–	–	–	1,520	–
HFM19	168.00	182.00	12010	2005-11-09	5.35	5.36	1.93	0.058	0.043	7.21	–	35.7	40.3	1.57	–	1,550	1,530
KFM01A	109.00	130.00	8913	2005-06-09	–	–	0.463	0.05	0.059	7.65	7.56	–	–	–	24.0	1,030	–
KFM01A	109.00	130.00	12008	2005-11-09	0.467	0.469	0.478	0.036	0.054	7.71	–	34.0	30.0	0.614	–	1,050	1,034
KFM02A	411.00	442.00	12002	2005-11-07	1.39	1.36	1.84	0.051	0.133	7.36	–	1.2	1.1	0.058	2.9	1,570	1,741
KFM02A	490.00	518.00	12004	2005-11-07	2.26	2.26	2.07	0.049	0.112	7.19	–	1.5	1.4	0.066	3.8	1,610	1,695
KFM03A	633.50	650.00	8926	2005-06-23	0.608	0.571	0.51	0.044	0.122	7.46	7.53	1.2	1.1	0.17	4.5	1,590	1,690
KFM03A	633.50	650.00	12001	2005-11-09	1.07	1.06	0.51	0.034	0.223	7.49	7.83	1.4	1.1	0.701	5.7	1,580	1,614
KFM03A	969.50	994.50	8927	2005-06-23	–	–	0.05	0.032	0.307	7.75	7.85	–	–	–	–	2,760	2,940
KFM03A	969.50	994.50	12005	2005-11-07	1.38	1.36	0.0894	0.028	0.63	6.27	–	2.0	1.0	0.838	2.8	2,760	2,830

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SICADA: water_composition

Idcode	Secup m	Seclow m	Sample no.	Sampling date	NH_4N mg/L	NO_2N mg/L	NO_3N mg/L	NO_2N/NO_3N mg/L	PO_4P mg/L	Temp. °C	P mg/L
HFM02	38.00	48.00	8915	2005-06-10	–	–	–	–	–	10.2	–
HFM02	38.00	48.00	12006	2005-11-09	0.548	< 0.0002	< 0.0003	< 0.0003	0.0174	7.7	0.0333
HFM04	58.00	66.00	8929	2005-06-23	–	–	–	–	–	7.8	–
HFM04	58.00	66.00	12003	2005-11-07	0.442	< 0.0002	< 0.0003	< 0.0003	0.0142	8.9	0.0254
HFM13	159.00	173.00	8916	2005-06-09	–	–	–	–	–	9.5	–
HFM13	159.00	173.00	12009	2005-11-09	1.42	< 0.0002	< 0.0003	< 0.0003	< 0.0005	8.1	< 0.0005
HFM15	85.00	95.00	8917	2005-06-09	–	–	–	–	–	9.6	–
HFM15	85.00	95.00	12007	2005-11-09	0.551	< 0.0002	< 0.0003	< 0.0003	0.0027	7.8	0.0175
HFM19	168.00	182.00	8914	2005-06-09	–	–	–	–	–	9.0	–
HFM19	168.00	182.00	12010	2005-11-09	2.07	< 0.0002	< 0.0003	< 0.0003	< 0.0005	7.6	0.0048
KFM01A	109.00	130.00	8913	2005-06-09	–	–	–	–	–	18.8	–
KFM01A	109.00	130.00	12008	2005-11-09	0.631	< 0.0002	< 0.0003	< 0.0003	0.0005	9.0	0.0009
KFM02A	411.00	442.00	12002	2005-11-07	1.62	0.0002	< 0.0003	< 0.0003	< 0.0005	9.3	< 0.0005
KFM02A	490.00	518.00	12004	2005-11-07	2.1	< 0.0002	< 0.0003	< 0.0003	< 0.0005	8.4	< 0.0005
KFM03A	633.50	650.00	8926	2005-06-23	0.246	< 0.0002	–	< 0.0003	0.0006	12.1	0.0033
KFM03A	633.50	650.00	12001	2005-11-09	0.404	< 0.0002	< 0.003	< 0.0003	0.0030	8.3	0.001
KFM03A	969.50	994.50	8927	2005-06-23	–	–	–	–	–	14.0	–
KFM03A	969.50	994.50	12005	2005-11-07	0.0008	< 0.002	0.0003	0.0003	0.0007	8.0	< 0.04

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SICADA: water_composition

Table A3-2. Trace elements.

Idcode	Secup m	Seclow m	Sample no.	Sampling date	U ug/L	Th ug/L	Ba ug/L	Ars 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
HFM02	38.00	48.00	12006	2005-11-09	11.2	< 0.02	243	0.13	< 0.05	0.0074	< 0.002	0.843	8.54	1.62	6.13	< 0.05	0.254
HFM04	58.00	66.00	12003	2005-11-07	3.18	0.0272	180	0.24	0.0602	0.0046	< 0.002	0.952	8.9	2.01	6.11	< 0.05	0.22
HFM13	159.00	173.00	12009	2005-11-09	16.2	< 0.2	553	< 1	< 0.5	< 0.05	< 0.002	0.0925	52.5	18.4	< 0.3	< 0.5	2.04
HFM15	85.00	95.00	12007	2005-11-09	18.1	0.0428	254	0.19	0.0937	< 0.004	< 0.002	1.14	12	2.190	12.9	< 0.05	0.266
HFM19	168.00	182.00	12010	2005-11-09	5.03	< 0.2	501	< 1	< 0.5	< 0.05	< 0.002	< 0.05	49.6	2.69	< 0.3	< 0.5	2.13
KFM01A	109.00	130.00	12008	2005-11-09	3.78	< 0.2	753	< 0.5	< 0.4	0.0274	< 0.002	0.0711	52.1	13.6	0.827	< 0.2	0.24
KFM02A	411.00	442.00	12002	2005-11-07	25.9	< 0.2	667	< 1	< 0.5	< 0.05	< 0.002	0.143	65.3	6.41	< 0.3	< 0.5	4.4
KFM02A	490.00	518.00	12004	2005-11-07	122	< 0.2	549	< 1	< 0.5	< 0.05	< 0.002	0.127	63	2.76	< 0.3	< 0.5	1.98
KFM03A	633.50	650.00	8926	2005-06-23	46.3	< 0.4	–	0.48	< 0.8	0.189	< 0.002	0.168	47.9	0.677	< 0.2	< 0.2	12.4
KFM03A	633.50	650.00	12001	2005-11-09	45.2	< 0.2	1,010	< 1	< 0.5	< 0.05	< 0.002	0.123	50	0.77	< 0.3	< 0.5	14
KFM03A	969.50	994.50	12005	2005-11-07	0.275	< 0.2	800	< 1	0.736	0.0966	0.0192	0.0557	36.2	0.896	< 0.3	< 0.5	0.563

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< "value" = below reporting limit
SICADA: trace_elements_1, trace_elements_2

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Ba ug/L	La ug/L	Hf ug/L	Tl ug/L	Ce ug/L	Pr ug/L	Nd ug/L	Sm ug/L	Eu ug/L	Gd ug/L	Tb ug/L	Dy ug/L	Ho ug/L
HFM02	38.00	48.00	12006	2005-11-09	49.9	0.043	0.0445	< 0.005	0.091	0.0127	0.0682	0.0308	0.0122	0.0884	< 0.05	0.155	0.0404
HFM04	58.00	66.00	12003	2005-11-07	35	0.117	0.0517	< 0.005	0.242	0.0319	0.151	0.0627	0.0138	0.129	< 0.05	0.2180	0.0538
HFM13	159.00	173.00	12009	2005-11-09	89.1	0.788	< 0.05	< 0.05	1.45	0.1930	1.0500	0.324	0.0595	0.8540	0.146	1.18	0.305
HFM15	85.00	95.00	12007	2005-11-09	67.1	0.181	0.103	< 0.005	0.331	0.0501	0.214	0.0771	0.0209	0.172	< 0.05	0.2590	0.0635
HFM19	168.00	182.00	12010	2005-11-09	72.3	0.0967	< 0.05	< 0.05	0.149	< 0.05	0.095	< 0.05	< 0.05	0.0999	< 0.05	0.134	< 0.05
KFM01A	109.00	130.00	12008	2005-11-09	399	0.87	< 0.02	< 0.03	1.25	0.157	0.887	0.257	0.0879	0.589	0.0907	0.8130	0.2270
KFM02A	411.00	442.00	12002	2005-11-07	85.2	0.48	< 0.05	< 0.05	0.67	0.07	0.38	0.0999	< 0.05	0.28	< 0.05	0.36	0.09
KFM02A	490.00	518.00	12004	2005-11-07	82.1	0.567	< 0.05	< 0.05	0.653	0.0599	0.243	< 0.05	< 0.05	0.109	< 0.05	0.108	< 0.05
KFM03A	633.50	650.00	8926	2005-06-23	151	0.464	< 0.04	< 0.2	0.425	0.0438	0.1760	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04	< 0.04
KFM03A	633.50	650.00	12001	2005-11-09	165	0.57	< 0.05	< 0.05	0.57	0.05	0.24	< 0.05	< 0.05	< 0.05	< 0.05	< 0.05	< 0.05
KFM03A	969.50	994.50	12005	2005-11-07	941	0.856	< 0.05	< 0.05	0.811	0.134	0.238	< 0.05	0.184	< 0.05	< 0.05	< 0.05	< 0.05

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SICADA: trace_elements_1, trace_elements_2

Idcode	Secup m	Seclow m	Sample no.	Sampling date	Er ug/L	Tm ug/L	Yb ug/L	Lu ug/L	Cr ug/L	Cu ug/L	Co ug/L	Ni ug/L	Mo ug/L	Pb ug/L	Zn ug/L	Sb ug/L
HFM02	38.00	48.00	12006	2005-11-09	0.152	0.0237	0.164	0.0293	0.119	< 0.1	0.035	0.327	8.48	< 0.01	< 0.2	0.0203
HFM04	58.00	66.00	12003	2005-11-07	0.198	0.0268	0.197	0.0332	0.167	< 0.1	0.021	0.254	4.51	0.0172	0.424	0.0103
HFM13	159.00	173.00	12009	2005-11-09	1.01	0.128	0.726	0.116	0.133	< 0.5	< 0.05	0.876	4.25	< 0.3	< 2	< 0.1
HFM15	85.00	95.00	12007	2005-11-09	0.2330	0.0313	0.217	0.0358	0.294	0.111	0.0422	0.404	7.34	0.0128	0.315	0.0194
HFM19	168.00	182.00	12010	2005-11-09	0.119	< 0.05	0.124	< 0.05	0.324	< 0.5	< 0.05	0.77	4.49	< 0.3	< 2	< 0.1
KFM01A	109.00	130.00	12008	2005-11-09	0.759	0.0852	0.478	0.0759	0.295	< 0.2	0.0711	0.567	35.9	< 0.1	< 0.8	< 0.1
KFM02A	411.00	442.00	12002	2005-11-07	0.26	< 0.05	0.17	< 0.05	0.184	< 0.5	0.392	1.19	22	< 0.3	< 2	0.131
KFM02A	490.00	518.00	12004	2005-11-07	0.0894	< 0.05	0.0585	< 0.05	0.173	0.539	1.03	2.64	48.1	< 0.3	< 2	< 0.1
KFM03A	633.50	650.00	8926	2005-06-23	< 0.04	< 0.04	< 0.04	< 0.04	0.598	< 0.4	0.0456	< 0.4	33.7	2.56	< 2	< 0.2
KFM03A	633.50	650.00	12001	2005-11-09	< 0.05	< 0.05	< 0.05	< 0.05	0.356	0.545	< 0.05	< 0.5	37.4	< 0.3	< 2	0.239
KFM03A	969.50	994.50	12005	2005-11-07	< 0.05	< 0.05	< 0.05	< 0.05	1.44	1.28	0.701	30.3	13	< 0.3	< 2	1.8

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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	δ^{2}H dev SMOW	^{3}H TU	δ^{18}O dev SMOW	^{10}B/^{11}B no unit	δ^{34}S dev CDT	δ^{13}C dev PDB	^{87}Sr/^{86}Sr no unit	^{14}C pmC	δ^{37}Cl dev SMOC
HFM02	38.00	48.00	8915	2005-06-10	–84.3	7.9	–11.6	0.2396	–	–	–	–	–
HFM02	38.00	48.00	12006	2005-11-09	–82.1	9.6	–82.1	0.2383	17.9	–11.70	0.724353	66.99	0.12
HFM04	58.00	66.00	8929	2005-06-23	–83.4	9.0	–11.8	–	–	–	–	–	–
HFM04	58.00	66.00	12003	2005-11-07	–84.4	10.6	–10.7	0.2385	13.4	–12.32	0.719551	73.00	0.34
HFM13	159.00	173.00	8916	2005-06-09	–72.5	–0.8	–9.50	0.2378	–	–	–	–	–
HFM13	159.00	173.00	12009	2005-11-09	–72.1	< 0.80	–9.50	0.2361	21.1	–5.75	0.717739	18.02	0.05
HFM15	85.00	95.00	8917	2005-06-09	–80.6	6.4	–11.1	0.2375	–	–	–	–	–
HFM15	85.00	95.00	12007	2005-11-09	–80.6	6.0	–9.40	0.2371	27.8	–11.22	0.721836	60.62	0.11
HFM19	168.00	182.00	8914	2005-06-09	–65.6	–0.8	–8.40	0.2371	–	–	–	–	–
HFM19	168.00	182.00	12010	2005-11-09	–65.1	1.0	–8.50	0.2352	25.0	–3.85	0.722525	30.90	0.10
KFM01A	109.00	130.00	8913	2005-06-09	–84.2	1.6	–11.2	0.2367	–	–	–	–	–
KFM01A	109.00	130.00	12008	2005-11-09	–87.4	1.3	–11.6	0.2364	15.6	–12.70	0.719771	46.1	0.19
KFM02A	411.00	442.00	12002	2005-11-07	–76.4	0.90	–10.0	0.2368	22.5	–5.45	0.716925	10.84	0.14
KFM02A	490.00	518.00	12004	2005-11-07	–66.2	0.90	–8.70	0.2369	21.9	–4.89	0.718172	17.33	0.02
KFM03A	969.50	994.50	8927	2005-06-23	–95.5	–0.8	–13.8	–	–	–	–	–	–
KFM03A	633.50	650.00	8926	2005-06-23	–80.7	1.5	–11.4	0.2345	23.6	xx	0.717501	xx	0.22
KFM03A	633.50	650.00	12001	2005-11-09	–83.5	0.80	–11.4	0.2362	25.1	xx	0.717380	xx	0.17
KFM03A	969.50	994.50	12005	2005-11-07	–97.8	< 0.80	–13.8	0.2372	29.1	xx	0.718715	xx	0.20

- = Not analysed
A = results will be reported later
xx = No result due to analytical problems
xxx = No result due to problem with the postal service.
< "value" = below reporting limit
SICADA: isotopes_1

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

Idcode	Secup m	Seclow m	Sample no.	Sampling date	^{238}U mBq/L	^{234}U mBq/L	^{230}Th mBq/L	^{226}Ra Bq/L	^{222}Rn Bq/L
HFM02	38.00	48.00	12006	2005-11-09	130	309	0.63	0.27	12.5
HFM04	58.00	66.00	12003	2005-11-07	37.7	114	2.9	0.18	120
HFM13	159.00	173.00	12009	2005-11-09	194	698	0.14	1.34	381
HFM15	85.00	95.00	12007	2005-11-09	225	452	0.77	0.3	52.4
HFM19	168.00	182.00	12010	2005-11-09	61	160	< 0.4	1.06	31.3
KFM01A	109.00	130.00	12008	2005-11-09	48.7	113	0.33	6.12	146
KFM02A	411.00	442.00	12002	2005-11-07	319	1260	0.39	4.1	400
KFM02A	490.00	518.00	12004	2005-11-07	1478	3020	0.32	3.5	1,350
KFM03A	633.50	650.00	8926	2005-06-23	490	742	< 0.23	0.32	2,900
KFM03A	633.50	650.00	12001	2005-11-09	530	816	0.44	23.2	3,530
KFM03A	969.50	994.50	12005	2005-11-07	4.1	9.9	0.31	14.1	13.0

- = Not analysed
A = Results will be reported later
x = No result due to sampling problems
xx = No result due to analytical problems
< "value" = below reporting limit
SICADA: u_th_isotope_t, ra_rn_isotope_t