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Site investigation SFR

Hydrogeochemical characterisation of groundwater in borehole KFR102A

Results from water sampling and analyses during March 2009

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July 2009

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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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Abstract

This report summarises the results from chemical investigations of groundwater in two sections of borehole KFR102A. The pumping sequences were c. 10 days in each section. The samples from KFR102A, sections 214–219 and 425–441 m borehole length (192–197 and 380–398 m.b.s.l.) were collected in March 2009 and yielded groundwater chemistry data in accordance with SKB chemistry class 4 and 5.

The chloride content was 4,180 and 3,501 mg/L and the flushing water content was 2.5 and 2.9% in sections 214–219 and 425–441 m borehole length, respectively. The relatively low flushing water contents and the stable water composition during the pumping and sampling periods indicate that the groundwaters are representative for the conditions in the two sampled borehole sections.

Also in borehole KFR102A, the water in the deepest borehole section was found to be less saline than the water in the more shallow section. The difference is clearly significant but not as striking as in the previously investigated borehole KFR101.

Sammanfattning

Denna rapport sammanfattar analysresultat från kemiska undersökningar av grundvatten i två sektioner av borrhål KFR102A. Pumpperioderna var cirka 10 dagar långa i båda sektionerna. Proven från KFR102A, sektionerna 214–219 och 425–441 m borrhålslängd (vertikalt djup 192–197 och 380–398 m) togs i mars 2009 och gav grundvattendata enligt SKB klass 4 och 5.

Kloridhalterna var 4 180 resprtvive 3 501 mg/L och spolvattenhalterna var 2,5 och 2,9 %, i sektionerna vid 214–219 och 425–441 m borrhålslängd. De relativt låga spolvattenhalterna och de stabila vattensammansättningarna under pumpnings- och provtagningsperioderna tyder på att grundvattnen är representativa för förhållandena i de två provtagna borrhålssektionerna.

Också i borrhålet KFR102A, visade det sig att vattnet i den djupaste borrhålssektionen var mindre salt än vattnet i den övre provtagna sektionen. Skillnaden är klart signifikant men ändå inte så påtaglig som i det tidigare undersökta borrhålet KFR101.

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1 Introduction

SKB is conducting investigations prior to a future enlargement of the SFR repository for low- and medium level nuclear waste situated close to Forsmark nuclear power plant in the Östhammar community. The investigations are performed in the area preliminary planned for the enlargement and are made according to the established geoscientific investigation program /1/. Borehole KFR102A was drilled in order to investigate the conditions at depth below the candidate volume for a future enlargement and to discover possible subhorizontal zones above the zone H2.

This document reports the performance and results from the hydrogeochemical sampling of groundwater in the core borehole KFR102A. The work was carried out in accordance with activity plan AP SFR-09-003. The controlling documents for performing this activity are listed in Table 1-1. Both activity plan and method documents are SKB:s internal controlling documents.

Original data from the reported activity are stored in the primary database Sicada and traceable in Sicada by the activity plan number (AP SFR-09-003). Only data in databases are accepted for further interpretation and modelling. The data presented in this report are regarded as copies of the original data. Data in the database may be revised, if needed. However, such revision of the database will not necessarily result in a revision of this report although the normal procedure is that major data revisions entail a reversion of the P-report. Minor revisions are normally presented as supplements, available at www.skb.se.

The hydrogeochemical investigation was performed during March 2009 and included water sampling and chemical analyses in section no. 2 and no. 5 in borehole KFR102A, see Table 1-2.

KFR102A is a SKB chemistry-type, telescopic and 600.83 m long borehole. A technical description and design of the borehole is presented in /2/. The drilling of the borehole was completed on December 12, 2008 and tap water was used as drilling water. Information on the drilling water composition is found in Appendix 1. The site investigation area in Forsmark as well as the location of the sampled borehole is shown in Figure 1-1.

Activity plan	Number	Version
Hydrogeokemisk karakterisering av grundvatten i borrhål KFR102A samt kompletterande provuttag/analyser i KFR101 och i tunnelborrhålen KFR02, KFR08, KFR56 och KFR7A.	AP SFR-09-003	1.0
Measurement system descriptions	Number	Version
Metodbeskrivning för vattenprovtagning och analys i instrumenterade borrhål.	SKB MD 425.001	1.0
Mätsystembeskrivning – Handhavandedel; System för hydrologisk och meterologisk datainsamling. Vattenprovtagning och utspädningsmätning i observationshål.	SKB MD 368.010	1.0
Provtagning och analys- kemilaboratorium.	SKB 452.001-019	1.0

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

Table 1-2. Borehole sections included in the hydrogeochemical sampling in March 2009 and corresponding transmissivity values.

Borehole section	Section borehole length [m]	Section elevation [m.b.s.l.]	Transmissivity [m²/s]
KFR102A:2	425–441	380–398	1.61E–06*
KFR102A:5	214–219	192–197	3.62E-07*

* Sicada (PFL measurements).



Figure 1-1. Overview of the SFR pier and the location of boreholes.

2 Objective and scope

The hydrogeochemical characterisation in the two borehole sections were conducted in order to obtain groundwater data from two more sampling locations that will contribute to the overall 3D picture of the groundwater conditions at the SFR site. The two selected borehole sections (214–219 m and 425–441 m borehole length; 192–197 and 380–398 m.b.s.l.) included flow anomalies located as far from each other as possible but still at a reasonable vertical depth. The unusual conditions observed in borehole KFR101, where the groundwater was much less saline at depth than in the shallower borehole section, was an additional motive for investigations in more than one section of the borehole. The analytical protocol includes sampling and analyses according to SKB chemistry class 4 and 5 as well as field measurements of pH, electrical conductivity and temperature.

3 Equipment

3.1 Sampling equipment

The sampled borehole KFR102A is equipped with 7 inflatable packers sealing off eight borehole sections of which two (sections no. 2 and no. 5) are used for water sampling. Outline of the instrumentation in a telescopic borehole is presented in Figure 3-1.

Pump equipment (GEOPUMP UV45) was used to retrieve the water samples from the sampled sections. An outline of the sampling setup is presented in Figure 3-2 and Figure 3-3 shows the lowering of the pump. The water passes through a coarse filter to eliminate large particles that may be present in the water, then through a by-pass tubing through the mini-packer which isolates the section and thereafter through the downhole pump on the way to the surface. The flow rate is controlled by varying the capacity of the downhole pump with a voltage regulator at the surface.



Figure 3-1. Instrumentation in telescopic core boreholes including circulation section used for sampling.



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.



Figure 3-3. Lowering of equipment in the water stand-pipe in order to pump water from the borehole section. From the bottom; filter, small inflatable packer and pump.

4 Performance

4.1 General

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

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, see chapter 6. The total volumes pumped from each section prior to sampling are given in Appendix 2. The pumping was for a short period performed simultaneously in the two sections, as no hydraulic connection between the sections was registered, see Appendix 3.

In addition to sampling of groundwater, field measurements of temperature, electric conductivity and pH were conducted. The water pumped from the borehole was led through a measurement cell with probes and electrodes as well as a temperature sensor for measurements of field pH (pH_F), field electrical conductivity (EC_F) and groundwater temperature.

Sample portions intended for analysis of major constituents and trace metals (by ICP technique), DOC, iron (by spectrometry) and nutrient salts were filtered on-line. Disposable 0.4 μ m 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.

4.3 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 4. The routines are applicable independently of sampling method or sampling object.

ldcode	Section [m]	Sampling Date	Sample no.	Analyses
KFR102A	425–441	09-03-11	16226	Class 4, ${}^{3}H$, $\delta^{2}H$ and $\delta^{18}O$, pH_F, EC_F and temp.
KFR102A	425–441	09-03-13	16227	Class 5, pH_F, EC_F and temp.
KFR102A	425–441	09-03-16	16228	Class 4, $^3H,\delta^2H$ and $\delta^{18}O,pH_F,EC_F$ and temp.
KFR102A	425–441	09-03-18	16232	Class 4, $^3H,\delta^2H$ and $\delta^{18}O,pH_F,EC_F$ and temp.
KFR102A	425–441	09-03-20	16233	Class 5 ⁺ , incl. U, Th, Ra and Rn isotopes, pH_F, EC_F and temp.
KFR102A	214–219	09-03-18	16234	Class 4, $^3H,\delta^2H$ and $\delta^{18}O,pH_F,EC_F$ and temp.
KFR102A	214–219	09-03-20	16235	Class 5, field measurement (pH_F, EC_F and water temperature).
KFR102A	214–219	09-03-23	16236	Class 4, $^3H,\delta^2H$ and $\delta^{18}O,pH_F,EC_F$ and temp.
KFR102A	214–219	09-03-25	16237	Class 4, $^3H,\delta^2H$ and $\delta^{18}O,pH_F,EC_F$ and temp.
KFR102A	214–219	09-03-27	16238	Class 5 ⁺ , incl. U, Th, Ra and Rn isotopes, pH_F, EC_F and temp.

Table 4-1. Samples and analytical protocol for KFR102A. Electrical conductivity, pH and water temperature are measured in the field (EC_F, pH_F and temp).

5 Nonconformities

Nonconformities have not been reported during the performance of this activity.

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.

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

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⁻, F⁻, I⁻, HS⁻ and NH₄⁺. Samples collected according to SKB chemistry class 5 include also P, 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.

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 $\pm 5\%$ in any of the cases. The basic water analysis data and relative charge balance errors are compiled in Appendix 1, Table A1-1.

The diagram in Figure 7-1 shows chloride concentrations versus EC values from previous investigations in Forsmark as well as from borehole KFR102A. The KFR102A data points follow the trend line indicating that the EC and chloride data sets are consistent.

Figure 7-2 presents the flushing water contents in the two sampled borehole sections, 214–219 m and 425–441 m borehole length (192–197 and 380–398 m.b.s.l.). The content should not exceed 1% in order for a sample to be considered fully representative for the groundwater of the sampled section, however contents below 5% are acceptable for most modelling purposes. This last condition was met in both borehole sections. The flushing water contents were relatively stable during the sampling periods.

The concentrations of chloride, calcium and sodium are presented in Figures 7-3 and 7-4. The concentrations of all major constituents remained constant in both borehole sections during the pumping and sampling periods.

The iron concentrations are compared in Figures 7-5 and 7-6. The determinations by ICP-AES (total Fe and spectrophotometry (Fe(II) and Fe-tot) agree well and the concentrations are stable through the sampling periods.

Sulphate analysed by ion chromatography (IC) is compared to sulphate determined as total sulphur by ICP-AES for sections 214–219 m and 425–441 m in Figures 7-7 and 7-8, respectively. The agreement between the two analysis methods (IC and ICP-AES) is rather good and the discrepancies correspond to the size of the analytical error.

7.1.2 Trace elements (rare earth metals and others)

The analyses of trace elements include Cr, Cu, Co, Ni, Mo, Pb, Zn, Sb, Al, U, Th, B, 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 1, Table A1-2. Due to low natural concentrations and frequent use in different equipments, the risk of contamination is high for common metals like Cr, Cu, Co, Ni, Mo, Zn and Al. Trace metal data exist for two samples from each borehole section and clear deviations between the two samples or enhanced values in both samples were obtained for the trace metals Cr, Cu, Zn and Al.

7.1.3 Stable and radioactive isotopes

The isotope determinations include the stable isotopes δ^2 H, 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 δ^2 H, δ^{18} O and 3 H. All other isotopes were determined twice (SKB class 5 sampling). Available isotope data are compiled in Appendix 1, Tables A1-3 and A1-4.



Figure 7-1. Chloride concentration versus electrical conductivity. Data from previous investigations at Forsmark are used to show the linear trend. Data from KFR102A are shown in pink.



Figure 7-2. Flushing water content in the groundwater samples from sections 214–219 m and 425–441 m borehole length.



Figure 7-3. Chloride, calcium and sodium concentrations in the groundwater samples from section 214–219 m.



Figure 7-4. Chloride, calcium and sodium concentrations in the groundwater samples from section 425–441 m.



Figure 7-5. Comparisons of iron concentrations obtained by ICP-AES and by spectrophotometry, section 214–219 m.



Figure 7-6. Comparisons of iron concentrations obtained by ICP-AES and by spectrophotometry, section 425–441 m.



Figure 7-7. Sulphate (SO4 by IC) compared to total sulphate calculated from total sulphur ($3 \times SO_{4}$ -S by ICP) versus date, section 214–219 m.



Figure 7-8. Sulphate (SO4 by IC) compared to total sulphate calculated from total sulphur (3×SO4-S by ICP) versus date, section 425–441 m.

8 Summary

The hydrogeochemical investigation in KFR102A in March 2009 included collection of five samples from each one of the two borehole sections at 214–219 and 425–441 m borehole length. Some observations regarding the performance and the results are listed below:

- The collected samples from both borehole sections showed relatively low flushing water contents (between 2 and 3%). Furthermore, the water compositions were very stable within each series.
- Pumping in section no. 2 and no. 5 did not cause any clear responses in the other borehole sections. There is a weak response in section no.1 during the pumping period in section no. 2 but this may be due to effects from the tubing. The absence of responses indicates that there is no short circuiting between the sections that can affect the samples.
- The water in the deepest borehole section was found to be less saline than the water in the more shallow section. The difference is clearly significant but not as striking as in borehole KFR101.
- The uranium concentrations are relatively high, especially in the deep section (20 μg/L).
- All the samples show sulphide concentrations below the detection limit. From previous investigations /3/ it has been suggested that the sulphide concentration (microbial production) could be affected by pumping. Heavy pumping was performed during and after the drilling and it cannot be excluded that the low concentrations are an artefact caused by the recent drilling and clean up pumping work.

9 References

- /1/ **SKB**, 2008. Geovetenskapligt undersökningsprogram för utbyggnad av SFR. SKB R-08-67, Svensk Kärnbränslehantering AB.
- /2/ Nilsson G, Ullberg A, 2009. Site investigation SFR, Drilling of the telescopic borehole KFR102A. SKB P-09-19, Svensk Kärnbränslehantering AB.
- /3/ Smellie J, Tullborg E-L, Nilsson A-C, Sandström B, Waber N, Gimeno M, Gascoyne M, 2008. Forsmark site investigation. Explorative analysis of major components and isotopes. In; B. Kalinowski (ed), 2008. SKB R-08-84, Svensk Kärnbränslehantering AB.

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Table A1-1. Water composition.

ldcode	Secup m	Seclow m	Sample no.	Sampling date	RCB %	Na mg/L	K mg/L	Ca mg/L	Mg mg/L	HCO₃ [⁻] mg/L	CI mg/L	SO4 ²⁻ mg/L	SO4-S mg/L	Br mg/l	F mg/L	Si mg/L	Fe mg/L	Fe-tot mg/L	Fell mg/L	Mn mg/L	Li mg/L	Sr mg/L
KFR102A	214	219	16234	2009-03-18	0.04	1,840	9.93	761	127	107	4,200	351	135	18.2	1.42	6.10	0.825	0.876	0.865	0.704	0.0563	12.5
KFR102A	214	219	16235	2009-03-20	0.27	1,850	9.43	763	125	107	4,200	354	131	17.7	1.42	5.97	0.735	0.759	0.762	0.697	0.0544	12.3
KFR102A	214	219	16236	2009-03-23	-1.52	1,740	9.34	773	122	107	4,200	355	131	18.8	1.47	5.91	0.708	0.693	0.689	0.701	0.0563	11.9
KFR102A	214	219	16237	2009-03-25	-1.37	1,720	9.67	775	126	105	4,170	356	132	18.7	1.52	6.01	0.718	0.742	0.738	0.703	0.0561	12.4
KFR102A	214	219	16238	2009-03-27	-1.07	1,750	9.51	773	124	105	4,180	356	132	19.4	1.48	6.09	0.753	0.764	0.767	0.699	0.0526	12.3
KFR102A	425	441	16226	2009-03-11	0.01	1,460	12.1	608	114	96.4	3,370	292	110	15.8	1.52	6.58	1.08	1.09	1.08	0.776	0.0463	8.63
KFR102A	425	441	16227	2009-03-13	-1.68	1,470	11.3	577	107	93.3	3,450	294	103	16.3	1.51	6.20	0.925	0.961	0.979	0.718	0.0443	8.50
KFR102A	425	441	16228	2009-03-16	-0.19	1,500	11.9	635	110	92.9	3,490	283	109	15.1	1.30	6.53	0.945	0.955	0.949	0.753	0.0460	9.34
KFR102A	425	441	16232	2009-03-18	-1.23	1,490	11.4	627	105	92.0	3,530	281	105	16.5	1.49	6.31	0.903	0.944	0.936	0.724	0.0464	9.28
KFR102A	425	441	16233	2009-03-20	0.75	1,540	11.7	657	108	90.6	3,510	285	109	16.8	1.44	6.45	0.936	0.942	0.949	0.742	0.0471	9.82
PFR000123	Drilling wa	ater	16173	2008-12-02	-0.94	28.8	1.64	35.5	2.14	83.6	6.6	73.1	28.0	<0.5	<0.5	2.83	-	-	-	-	<0.004	0.045

ldcode	Secup m	Seclow m	Sample no.	Sampling date	l [`] mg/L	pH _L	pH_F	DOC mg/L	TOC mg/L	HS ⁻ mg/L	Drill water %	Uranine µg/L	EC_L mS/m	EC_F mS/m	NH₄N mg/L	NO₂N mg/L	NO₃N mg/L	NO₂N+NO₃N mg/L	PO₄P mg/L	P mg/L	Temp ℃
KFR102A	214	219	16234	2009-03-18	0.112	7.58	7.61	1.7	1.8	<0.02	2.48	5.20	1,230	1,248	0.123	-	-	0.0006	<0.0005	-	5.4
KFR102A	214	219	16235	2009-03-20	0.107	7.53	7.69	1.6	1.6	<0.02	2.55	5.35	1,230	1,247	0.109	<0.0002	х	x	< 0.0005	<0.0005	5.1
KFR102A	214	219	16236	2009-03-23	0.116	7.57	7.70	1.5	1.6	<0.02	2.62	5.50	1,260	1,249	0.122	-	-	0.0017	< 0.0005	-	5.0
KFR102A	214	219	16237	2009-03-25	0.110	7.59	7.70	1.5	1.6	<0.02	2.71	5.70	1,270	1,241	0.114	-	-	0.0019	< 0.0005	-	5.3
KFR102A	214	219	16238	2009-03-27	0.110	7.58	7.54	1.5	1.5	<0.02	2.48	5.20	1,270	1,241	0.107	<0.0002	0.0008	0.0008	< 0.0005	< 0.0005	5.5
KFR102A	425	441	16226	2009-03-11	0.0665	7.58	7.89	1.8	1.8	<0.02	2.38	5.00	1,040	1,027	0.193	-	-	0.0007	< 0.0005	-	5.7
KFR102A	425	441	16227	2009-03-13	0.0866	7.54	7.86	1.7	1.7	<0.02	2.38	5.00	1,040	1,038	0.173	< 0.0002	0.0015	0.0015	< 0.0005	< 0.0005	6.0
KFR102A	425	441	16228	2009-03-16	0.0695	7.51	7.65	1.6	1.6	<0.02	2.55	5.35	1,050	1,049	0.174	-	-	0.0034	< 0.0005	-	5.8
KFR102A	425	441	16232	2009-03-18	0.0833	7.51	7.65	1.6	1.6	<0.02	2.74	5.75	1,050	1,050	0.174	-	-	0.0031	< 0.0005	-	4.9
KFR102A	425	441	16233	2009-03-20	0.0783	7.49	7.73	1.6	1.6	<0.02	2.86	6.00	1,052	1,054	0.155	<0.0002	0.0014	0.0014	<0.0005	<0.0005	5.1
PFR000123	B Drilling	y water	16173	2008-12-02	-	8.11	-	-	-	-	-	-	33.6	-	-	-	-	-	-	-	-

– = Not analysed.

pH_L; EC_L = Lab. measurem. of pH and EC.

pH_F; EC_F = Field measurem. of pH and EC.

< "value" = value below reporting limit.

x = no result due to sampling problems.

RCB% = Rel. charge balance error %.

Sicada: water_composition.

Table A1-2. Trace elements.

ldcode	Secup m	Seclow m	Sample no.	Sampling date	U ug/L	Th ug/L	B ug/L	As ug/L	Sc ug/L	Cd ug/L	Hg ug/L	V ug/L	Rb ug/L	Y ug/L	Zr ug/L	ln ug/L	Cs ug/L
KFR102A	214	219	16235	2009-03-20	6.07	<0.2	927	<0.5	<0.4	<0.02	<0.002	0.0705	23.3	3.47	<0.1	<0.2	0.765
KFR102A	214	219	16238	2009-03-27	6.38	<0.2	924	<0.5	<0.4	< 0.02	<0.002	0.112	23.0	3.87	<0.1	<0.2	0.716
KFR102A	425	441	16227	2009-03-13	21.7	<0.2	788	0.550	<0.4	0.0220	<0.002	0.139	23.9	1.76	<0.1	<0.2	0.676
KFR102A	425	441	16233	2009-03-20	20.5	<0.2	886	<0.5	<0.4	<0.02	<0.002	0.0701	22.5	1.68	<0.1	<0.2	0.630
ldcode	Secup m	Seclow m	Sample no.	Sampling date	Ba ug/L	La ug/L	Hf ug/L	TI 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
KFR102A	214	219	16235	2009-03-20	127	0.201	<0.02	<0.05	0.290	0.0353	0.263	0.0645	0.0233	0.1290	<0.02	0.151	0.0458
KFR102A	214	219	16238	2009-03-27	126	0.313	<0.02	<0.05	0.531	0.0875	0.449	0.1180	0.0321	0.2090	0.0298	0.226	0.0626
KFR102A	425	441	16227	2009-03-13	106	0.114	<0.02	<0.05	0.189	0.0235	0.124	0.0251	<0.02	0.0565	<0.02	0.0613	<0.02
KFR102A	425	441	16233	2009-03-20	113	0.0994	<0.02	<0.05	0.161	0.0205	0.108	0.0277	<0.02	0.0570	<0.02	0.0625	<0.02
ldcode	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	Al µg/L
KFR102A	214	219	16235	2009-03-20	0.158	<0.02	0.108	<0.02	0.546	<0.2	0.0882	0.658	5.82	<0.1	12.1	<0.1	7.68
KFR102A	214	219	16238	2009-03-27	0.190	0.0239	0.141	0.0222	1.18	2.14	0.0782	0.730	5.84	0.120	11.8	0.107	28.5
KFR102A	425	441	16227	2009-03-13	0.066	<0.02	0.0542	<0.02	3.00	1.18	0.462	2.03	7.60	0.133	329	0.109	70.1
KFR102A	425	441	16233	2009-03-20	0.0668	<0.02	0.0517	<0.02	0.412	0.213	0.410	1.16	7.09	<0.1	306	<0.1	7.07

Table A1-3.	Isotopes I.

ldcode	Secup m	Seclow m	Sample no	Sampling date	δ²H dev SMOW	³H TU	$\delta^{18}O$ dev SMOW	¹⁰ B/ ¹¹ B no unit	δ³⁴S dev CDT	δ¹³C dev PDB	⁸⁷ Sr/ ⁸⁶ Sr no unit	^{1₄} C pmC	δ³7CI dev SMOC
KFR102A	214	219	16234	2009-03-18	-75.3	2.3	-10.0	_	_	_	_	_	_
KFR102A	214	219	16235	2009-03-20	-74.9	1.8	-10.1	0.2369	11.6	-7.92	0.716605	А	А
KFR102A	214	219	16236	2009-03-23	-73.7	2.7	-10.0	-	_	-	-	-	_
KFR102A	214	219	16237	2009-03-25	-75.9	2.9	-10.1		-	-	-	-	_
KFR102A	214	219	16238	2009-03-27	-77.8	2.9	-10.2	0.2363	12.0	-8.17	0.716610	А	А
KFR102A	425	441	16226	2009-03-11	-87.5	3.7	-11.5	_	-	-	-	-	_
KFR102A	425	441	16227	2009-03-13	-87.1	3.8	-11.5	0.2368	11.6	-8.28	0.7167	А	А
KFR102A	425	441	16228	2009-03-16	-85.0	3.2	-11.4	_	-	-	-	-	_
KFR102A	425	441	16232	2009-03-18	-85.1	4.5	-11.4	_	-	-	-	-	_
KFR102A	425	441	16233	2009-03-20	-86.1	4.2	-11.4	0.2373	12.1	-8.34	0.716675	А	А
PFR000123	Drilling v	vater	16173	2008-12-02	-73.1	_	-9.60	_	_	_	_	_	_

A = Not reported from laboratory at printing date.

Table A1-4. Isotopes II.

ldcode	Secup m	Seclow m	Sample no.	Sampling date	²³⁸ U mBq/kg	²³⁵ U mBq/kg	²³⁴ U mBq/kg	²³⁰ Th mBq/kg	²³² Th mBq/kg	²²⁶ Ra Bq/L	²²² Rn Bq/L At time of analysis	²²² Rn Bq/L At time of collection
KFR102A	214	219	16238	2009-03-27	76.0	2.8	282	0.39	0.31	1.92	624	1,446
KFR102A	425	441	16233	2009-03-20	257	10.4	628	0.10	0.10	1.09	124	450

Sampling information

Idcode section	Tube volume [dm ³]	Section volume [dm ³]	Total volume [dm ³]	Pumping time	Flow rate [mL/min]	Pumped volume [dm ^³]	Sampling date	Sample no.	Pressure responses in other sections of the borehole
KFR102A:2	22.7	27.4	50.1	23 h 2 min	160	221	2009-03-11	16226	No
"	"	"	"	47 h 53 min	210	824	2009-03-13	16227	No
"	"	"	"	71 h 32 min	210	1,726	2009-03-16	16228	No
"	"	"	"	48 h 17 min	210	2,333	2009-03-18	16232	No
"	"	"	"	46 h 42 min	190	2,865	2009-03-20	16233	No
KFR102A:5	20.1	8.4	28.5	47 h 29 min	90	256	2009-03-18	16234	No
"	"	"	"	47 h 12 min	190	794	2009-03-20	16235	No
"	"	"	"	72 h 55 min	210	1,713	2009-03-23	16236	No
"	"	"	"	48 h 5 min	220	2,354	2009-03-25	16237	No
"	"	"	"	47 h 35 min	210	2,953	2009-03-27	16238	No

Pressure registrations in KFR102A during pumping and sampling, HMS system



Sampling and analytical methods

Table A4-1. 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, SO₄, Br, F⁻, I⁻	Plastic	100	Yes (not in the field)	No	Titration (Cl⁻) IC (Cl⁻, SO4, 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), 3 Si(tot), Li, Sr	Plastic (at low conc. acid washed bottles)	100	Yes (not in the field)	Yes (not in the field, 1 mL HNO₃)	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 HNO₃)	ICP-AES ICP-MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic (Acid washed)	500	Yes	Yes (5 mL HCI))	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
Total organic Carbon	ТОС	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)

Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/ conservation*	Analysis method	Analysis within – or delivery time to lab.
Tritium,	³ H (enhanced.)	Plastic (dry bottle) Plastic	500	No	-	LSC	Not critical (month)
Chlorine-37	Chlorine-37		100	No	-	MS	
Carbon isotopes	¹³ C, ¹⁴ C	Glass (brown)	100×2	No	-	(A)MS	A few days
Sulphur isotopes	³⁴ S	Plastic	500-1,000	Yes	-	Combustion, MS	No limit
Strontium-isotopes	⁸⁷ Sr/ ⁸⁶ Sr	Plastic	100	Yes	-	TIMS	Days or Week
Uranium and Thorium isotopes	²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th,	Plastic	50	No	-	Alfa spectroscopy	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	No	No	LSS	Immediate transport
Dissolved gas (content and composition)	$\begin{array}{l} \text{Ar, } N_2, \text{CO}_2, \text{O}_2, \text{CH}_4, \text{H}_2, \\ \text{CO, } C_2\text{H}_2, \text{C}_2\text{H}_4, \text{C}_2\text{H}_6, \text{C}_3\text{H}_8 \end{array}$	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series and fractionation (see below)	Polycarbonate filter	0.45, 0.2 and 0.05 μm	-	N ₂ atmosphere	ICP-AES ICP-MS	Immediate transport
Humic and fulvic acids	Fractionation	Fractions are collected in plastic bottles	250	-	N ₂ atmosphere	UV oxidation, IR (DOC)	Immediate transport
Archive samples with acid	-	Plast (washed in acid)	100×2 **	Yes	Yes (1 mL HNO ₃)	-	Storage in freeze container
Archive samples without acid	-	Plastic	250×2 **	Yes	No	-	Storage in freeze container
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	Yes (in the field)	No, frozen immediately***	Spectrophotometry	Short transportation time
Total concentrations of Nitrogen and Phosphorous	N-tot, P-tot	Plastic	100	No	No, frozen immediately***	Spectrophotometry	Short transportation time
Particulate Carbon, Nitrogen and Phosphorous	POC, PON, POP	Plastic	1,000	Yes (within 4 h) prepared filters. Blank filters	Filtering, the filters are frozen immediately 2 filters/sample	Elementar-analysator (N, C) own method 990121 (P)	Short transportation time
Chlorophyll	Chlorophyll a, c and pheopigment	Plastic	1,000–2,000	Yes (within 4 h)	Filtering, the filters are frozen immediately	Spectrophotometry Fluorometry	Short transportation time
Oxygen	Dissolved O ₂	Winkler, glass	2×ca 120	No	Mn (II) reagent lodide 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
MS	Mass Spectrometry
TIMS	Thermal Ionization Mass Spectrometer
LSC	Liquid Scintillation Counting
(A)MS	(Accelerator) Mass Spectrometry
GC	Gas Chromatography
LSS	Liquid Scintillation Spectroscopy

A4-2. Reporting limits and measurement uncertainties, updated 2008.

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
рН	Potentiometric	3–10	pH unit	±0.1
EC	Electrical Conductivity meas.	1–150 150–10,000	mS/m	5% 3%
HCO₃	Alkalinity titration	1	mg/L	4%
C⊢ C⊢	Mohr-titration IC	≥70 0.5–70	mg/L	5% 8%
SO ₄	IC	0.5	mg/L	12%
Br	IC	DL 0.2, RL 0.5	mg/L	15%
Br	ICP SFMS	0.001, 0.004, 0.010 ⁴	mg/L	25% ⁵
F- F-	IC Potentiometric	DL 0.2, RL 0.5 DL 0.1, RL 0.2	mg/L	13% 12%
I-	ICP SFMS	0.001, 0.004, 0.010 4	mg/L	25% ⁵
Na	ICP AES	0.1	mg/L	13%
К	ICP AES	0.4	mg/L	12%
Са	ICP AES	0.1	mg/L	12%
Mg	ICP AES	0.09	mg/L	12%
S(tot)	ICP AES	0.16	mg/L	12%
Si(tot)	ICP AES	0.03	mg/L	14%
Sr	ICP AES	0.002	mg/L	12%
Li	ICP AES	0.004	mg/L	12.2%
Fe	ICP AES	0.02	mg/L	13.3% ⁶
Fe	ICP SFMS	0.0004, 0.002, 0.004 4	mg/L	20% 6
Mn	ICP AES	0.003	mg/L	12.1% 5
Mn	ICP SFMS	0.00003, 0.00004, 0.0001 4	mg/L	53% ⁶
Fe(II), Fe(tot)	Spectrophotometry	DL 0.006, RL 0.02	mg/L	0.005 (0.02–0.05 mg/L) 9% (0.05–1 mg/L) 7% (1–3 mg/L)
HS⁻	Spectrophotometry, SKB	SKB DL 0.006, RL 0.02	mg/L	25%
HS⁻	Spectrophotometry, external laboratory	0.01	mg/L	0.02 (0.01–0.2 mg/L) 12% (>0.2 mg/L)
NO_2 as N	Spectrophotometry	0.1	μg/L	2%
NO₃ as N	Spectrophotometry	0.2	μg/L	5%
NO_2 + NO_3 as N	Spectrophotometry	0.2	μg/L	0.2 (0.2–20 μg/L) 2% (>20 μg/L)
NH₄ as N	Spectrophotometry, SKB	11	μg/L	30% (11–20 μg/L) 25% (20–50 μg/L) 12% (50–1,200 μg/L)
NH₄ as N	Spectrophotometry external laboratory	0.8	μg/L	0.8 (0.8–20 μg/L) 5% (>20 μg/L)

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
PO₄ as P	Spectrophotometry	0.7	μg/L	0.7 (0.7–20 μg/L) 3% (>20 μg/L)
SiO ₄	Spectrophotometry	1	μg/L	2.5% (>100 μg/L)
O ₂	Iodometric titration	0.2–20	mg/L	5%
Chlorophyll a, c pheopigment ⁷	/1/	0.5	μg/L	5%
PON 7	/1/	0.5	μg/L	5%
POP 7	/1/	0.1	μg/L	5%
POC 7	/1/	1	μg/L	4%
Tot-N ⁷	/1/	10	μg/L	4%
Tot-P ⁷	/1/	0.5	μg/L	6%
AI,	ICP SFMS	0.2, 0.3, 0.7 4	μg/L	17.6% ⁶
Zn	ICP SFMS	0.2, 0.8, 2 4	μg/L	15.5, 17.7, 25.5% ⁶
Ba, Cr, Mo,	ICP SFMS	0.01, 0.04, 0.1 4	μg/L	Ba 15%⁴, Cr 22%⁵ Mo 39% ⁶
Pb	ICP SFMS	0.01, 0.1, 0.3 4	μg/L	15% ⁶
Cd	ICP SFMS	0.002, 0.02, 0.5 4	μg/L	15.5% ⁶
Hq	ICP AFS	0.002	ua/L	10.7% 6
Co	ICP SFMS	0.005. 0.02. 0.05 4	ua/L	25.9% ⁶
V	ICP SFMS	0.005. 0.03. 0.05 4	µa/L	18.1% ⁶
Cu	ICP SFMS	0.1. 0.2. 0.5 4	µa/L	14.4% ⁶
Ni	ICP SFMS	0.05. 0.2. 0.5 4	µa/L	15.8% ⁶
P	ICP SFMS	1, 5, 40 ⁴	μg/l	16.3% ⁶
As	ICP SEMS	0.01 (520 mS/m)	μg/l	59 2% ⁶
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu	ICP SFMS	0.005, 0.02, 0.05 4	μg/L	20%, 20%, 25% ⁶
Sc, In, Th	ICP SFMS	0.05, 0.2, 0.5 ⁴	μg/L	25% ⁶
Rb, Zr, Sb, Cs	ICP SFMS	0.025, 0.1, 0.25 4	μg/L	15%, 20%, 20% ⁵ 25% ⁶
TI	ICP SFMS	0.025, 0.1, 0.25 4	μg/L	14.3% ^{5 and 6}
Y, Hf	ICP SFMS	0.005, 0.02, 0.05 4	μg/L	15%, 20%, 20% ⁵ 25% ⁶
U	ICP SFMS	0.001, 0.005, 0.01 ⁴	μg/L	13.5%, 14.3%, 15.9% ⁵ 19.1%, 17.9%, 20.9% ⁶
DOC	UV oxidation, IR Carbon analysator	0.5	mg/L	8%
TOC	UV oxidation, IR Carbon analysator	0.5	mg/L	10%
δ²H	MS	2	% SMOW 8	0.9 (one standard deviation)
δ 18Ο	MS	0.1	% SMOW 8	0.1 (one standard dev.)
³Н	LSC	0.8	TU ⁹	0.8
δ ³⁷ Cl	A (MS)	0.2	‰ SMOC 10	0.2 17
δ13C	A (MS)	-	% PDB 11	0.3 17
¹⁴ C pmc	A (MS)	-	PMC ¹²	0.4 17
δ ³⁴ S	MS	0.2	‰ CDT ¹³	0.4 (one standard dev.)
⁸⁷ Sr/ ⁸⁶ Sr	TIMS	-	No unit (ratio) ¹⁴	0.00002
¹⁰ B/ ¹¹ B	ICP SFMS	-	No unit (ratio) ¹⁴	-
²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th	Alfa spectr.	0.0001	Bq/L ¹⁵	≤5% (Counting statistics uncertainty)
²²² Rn, ²²⁶ Ra	LSS	0.015	Bq/L	≤5% (Count. stat. uncert.)

¹ Many elements may be determined by more than one ICP technique depending on concentration range. The most relevant technique and measurement uncertainty for the concentrations normally encountered in groundwater are presented. In cases where two techniques were frequently used, both are displayed.

² Reporting limits (RL), generally 10×standard deviation, if nothing else is stated. Measured values below RL or DL are stored as negative values in Sicada (i.e. –RL value and –DL value).

³ Measurement uncertainty reported by the laboratory, generally as ± percent of measured value in question at 95% confidence interval.

⁴ Reporting limits at electrical cond. 520 mS/m, 1,440 mS/m and 3,810 mS/m respectively.

⁵ Measurement uncertainty at concentrations 100×RL.

⁶ Measurement uncertainty at concentrations 10×RL.

⁷ Determined only in surface waters. PON, POP and POC refers to Particulate Organic Nitrogen, Phosphorous and Carbon, respectively.

⁸ Per mille deviation¹⁶ from SMOW (Standard Mean Oceanic Water).

⁹ TU = Tritium Units, where one TU corresponds to a tritium/hydrogen ratio of 10⁻¹⁸ (1 Bq/L Tritium = 8.45 TU).

¹⁰ Per mille deviation¹⁶ from SMOC (Standard Mean Oceanic Chloride).

¹¹ Per mille deviation¹⁶ from PDB (the standard PeeDee Belemnite).

¹² The following relation is valid between pmC (percent modern carbon) and Carbon-14 age: pmC = $100 \times e^{((1950-y-1.03t)/8274)}$ where y = the year of the C-14 measurement and t = C-14 age.

^{13.}Per mille deviation¹⁶ from CDT (the standard Canyon Diablo Troilite).

¹⁴ Isotope ratio without unit.

¹⁵ The following expressions are applicable to convert activity to concentration, for uranium-238 and thorium-232:

1 ppm U = 12.4 Bq/kg²³⁸U, 1 ppm Th = 3.93 Bq/kg²³²Th.

¹⁶ Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as:

δyl = 1,000×(Ksample-Kstandard)/Kstandard, where K = the isotope ratio and yl = 2H, 18O, 37Cl, 13C or 34S etc.

¹⁷ SKB estimation from duplicate analyses by the contracted laboratory.