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Forsmark site investigation

Sampling and analysis of precipitation, September 2005 to June 2007

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December 2007

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Abstract

Sampling and analyses of precipitation within the ongoing long term hydrochemical monitoring programme in Forsmark is reported for the period September 2005 to June 2007.

The analytical protocol included major constituents such as Na, K, Ca, Mg, Fe, Br⁻, Cl⁻, SO₄-S and HCO₃⁻ as well as measurements of pH and electrical conductivity. Furthermore, the trace metal aluminium and the isotopes tritium (³H), deuterium (δD) and oxygen-18 (δ¹⁸O) were determined.

Precipitation collectors were placed at a regular sampling point close to the candidate area at the Forsmark site and at a distant reference sampling point in the middle of Sweden, in Sjötorp at the Lake Vänern. The reference point was positioned at a long distance from any nuclear power plant and was sampled for tritium analyses.

Sammanfattning

Provtagning och analyser av nederbörd inom det pågående hydrokemiska monitoringsprogrammet för långtidsövervakning i Forsmark rapporteras för perioden september 2005 till Juni 2007.

Analysprogrammet omfattade huvudkomponenter som Na, K, Ca, Mg, Fe, Br⁻, Cl⁻, SO₄-S och HCO₃⁻ samt mätningar av pH och elektrisk konduktivitet. Vidare bestämdes spårmetallen aluminium och isotoperna tritium (³H), deuterium (δ D) och syre-18 (δ^{18} O).

Utrustning för insamling av nederbörd placerades vid en ordinarie provpunkt inom kandidatområdet i Forsmark och vid en avlägsen referenspunkt mitt i Sverige, i Sjötorp vid sjön Vänern. Referenspunkten valdes på ett stort avstånd från alla kärnkraftverk och provtogs för tritiumanalyser.

Contents

1	Introduction	7
2	Objective and scope	9
3	Equipment	11
4	Performance	13
4.1	Sampling	13
	4.1.1 Sampling during summer	13
	4.1.2 Sampling during winter	14
4.2	Sample treatment and chemical analyses	14
4.3	Data handling	14
4.4	Nonconformities	15
5	Results	17
5.1	Basic water analyses	17
5.2	Isotope analysis	17
6	Summary and discussions	19
	References	21
	Appendix 1 Sampling and analytical methods	23
	Appendix 2 Compilation of water analysis data	29

1 Introduction

This document reports the performance and the results of the activity “Hydrochemical monitoring of precipitation”, which is one of the activities performed within the site investigation at Forsmark /1/. The work was carried out in accordance with activity plans AP PF 400-05-090 and AP PF 400-07-001. In Table 1-1 controlling documents for conducting this activity are listed. Both activity plans and method descriptions are SKB’s internal controlling documents.

Precipitation was collected at the sampler location PFM002564. The position of the samplers is shown in Figure 1-1. In 2006, the reference point for tritium analyses PFM102271 was introduced to the programme. This point is located in Sjötorp, at Lake Vänern.

Original data from the reported activity are stored in the primary database Sicada. Data are traceable in Sicada by the Activity Plan number . 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 databases may be revised, if needed. Such revisions will not necessarily result in a revision of the P-report, although the normal procedure is that major data revisions entail a revision of the P-report. Minor revisions are normally presented as supplements, available at www.skb.se.

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

Activity plan	Number	Version
Hydrokemiskt övervakningsprogram för nederbörd	AP PF 400-05-090	1.0
Hydrokemiskt övervakningsprogram för nederbörd 2007	AP PF 400-07-001	1.0
Method description	Number	Version
Provtagning och analys av nederbörd	SKB MD 423.003	2.0

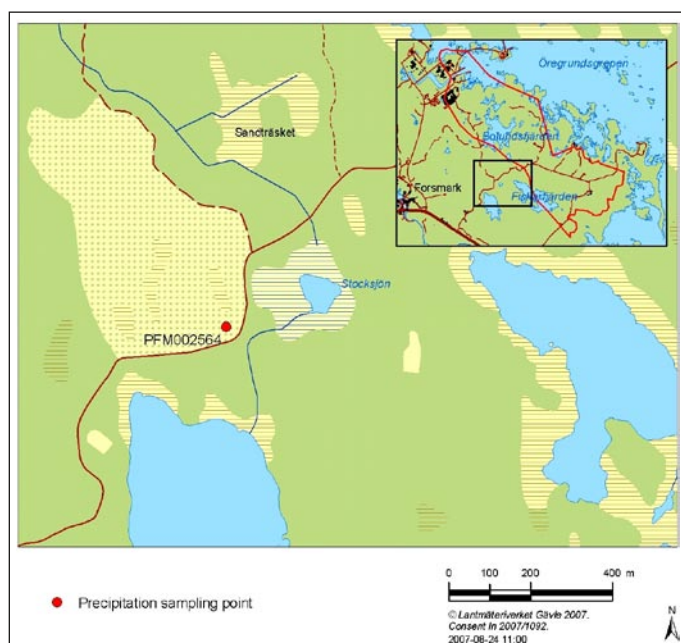


Figure 1-1. Location of the samplers for precipitation, PFM002564, within the Forsmark investigation area.

2 Objective and scope

Information on the chemical composition of precipitation and its variation in Forsmark is useful in the following contexts:

- to improve the understanding of groundwater formation and other hydrogeological conditions at the site,
- as boundary conditions for chemical modelling purposes,
- possible use as reference water in mixing calculations.

Sampling and analysis of precipitation are mainly performed according to the SKB class 3 /2/. However, aluminium and iron are also included in the analytical protocol.

Besides the regular sampling point within the site investigation area in Forsmark, a reference point for tritium samples was introduced in August 2006. This point, PFM102271, is located in Sjötorp close to the lake Vänern and was selected due to the long distance to any nuclear power plant. It was observed that the tritium content in precipitation and surface waters close to the nuclear power plants at Oskarshamn and Forsmark varied more than expected and a possible reason was occasional contamination from the power plants. Therefore, samples from an inland position were needed for comparison.

3 Equipment

Two different types of samplers for precipitation were used during the reported monitoring period. The first type /2/ was used until April 2007 and was initially delivered from IVL (Institutet för vatten och luftvård), see Figure 3-1. A second type (delivered from NILU, Norway) was used for the sample collected during May–June 2007, see Figure 3-2. Both sampling equipments consisted of a summer and a winter setup. The new winter setup was not used during the sampling period.



Figure 3-1. a) One out of five summer setups of the precipitations samplers used until April 2007. Five setups were used in order to increase the collected sample volume. b) One out of five winter setups of the precipitations samplers used until April 2007.



Figure 3-2. The new precipitation samplers (summer setup) used from May 2007 at Forsmark. Two sampler setups were used in order to increase the collected volume of precipitation.

4 Performance

4.1 Sampling

Sampling of precipitation within the Forsmark area was carried out according to activity plans AP PF 400-05-090 and AP PF 400-07-001 following the method description SKB MD 423.003 (Provtagning och analys av nederbörd), all SKB internal controlling documents.

4.1.1 Sampling during summer

The risk for biased isotope analyses due to evaporation was considered by more frequent collection of precipitation water from the field during summer time and by the use of samples bottles with narrow necks. The sampler bottles were removed from their stands every week and the contents pooled together with water from previous weeks and stored in a refrigerator. The collected precipitation from a two months period was then pooled into one large bottle and portioned into smaller bottles for distribution to the different analytical laboratories, see Figure 4-1, for a schematic outline of the sampling procedure. The bottles belonging to the old equipment were used together with thin plastic bags inside them, which were replaced after each sampling.

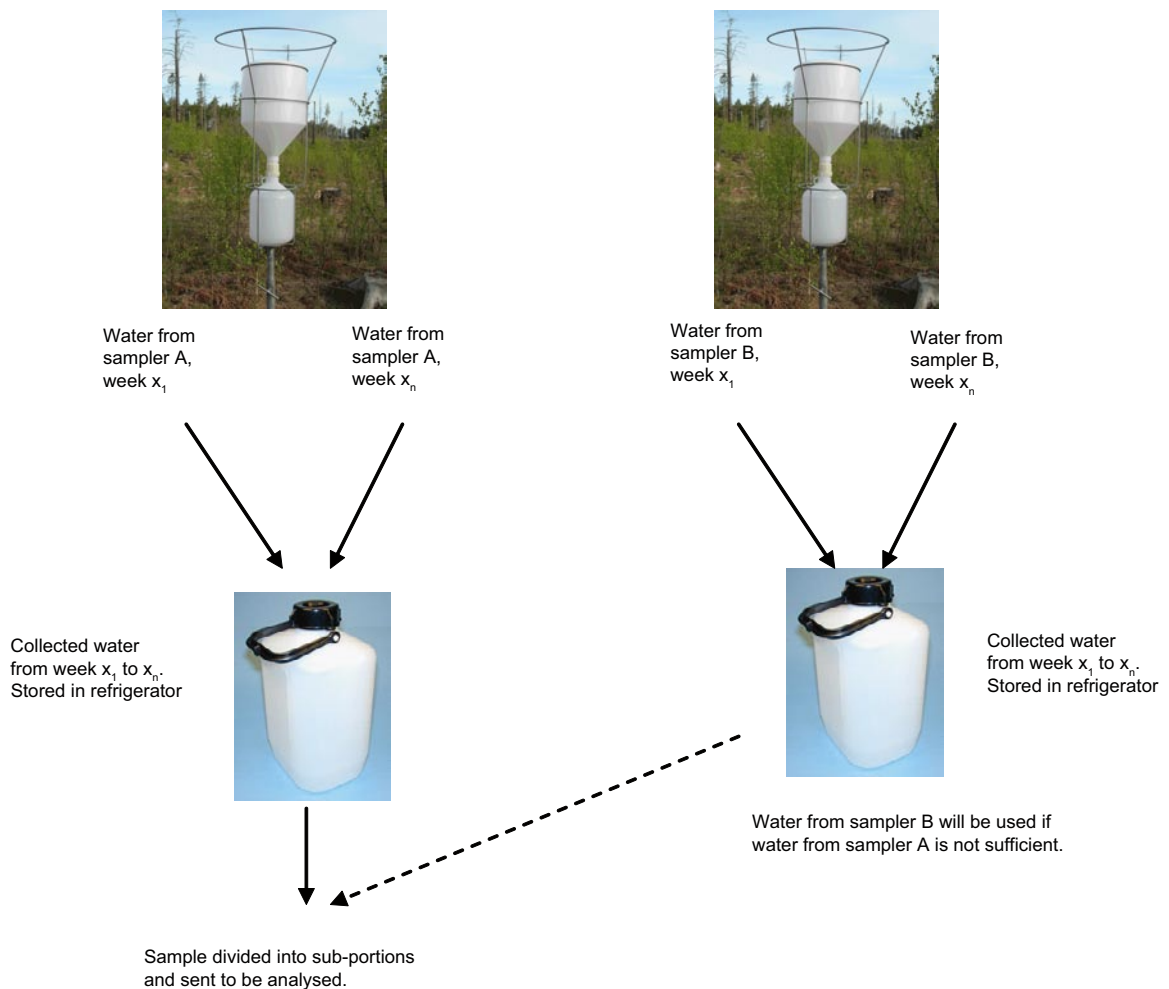


Figure 4-1. Schematic outline for collection of precipitation samples.

4.1.2 Sampling during winter

During winter time the samplers were fetched every second week and placed indoors in order to let the snow melt into the sampling bottles. Otherwise, the procedure was the same as for the summer samples.

4.2 Sample treatment and chemical analyses

An overview of sample treatment and analysis routines is given in Appendix 1. The routines are applicable independent of sampling method or type of sampling object. The sub-samples and analyses are listed in Table 4-1.

4.3 Data handling

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

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 raw data tables for further evaluation. The evaluation results in a final reduced data set for each sample. These data sets are compiled in a primary data table named “water_composition”. The evaluation is based on:

- Comparison of the results from different laboratories and/or methods. The analyses are repeated if a large disparity is noted (generally more than 10%).
- Calculation of charge balance errors. Relative errors within $\pm 5\%$ are considered acceptable (in surface waters $\pm 10\%$).

$$rel.error(\%) = 100 \times \frac{\sum cation(equivalents) - \sum anions(equivalents)}{\sum cation(equivalents) + \sum anion(equivalents)}$$

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

All results from *special analyses of trace metals and isotopes* are inserted directly into primary data tables. In those cases where the analyses are repeated or performed by more than one laboratory, a “best choice” notation will indicate those results which are considered most reliable. An overview of the data management is given in Figure 4-2.

Table 4-1. Sampling volumes and analysed components.

Sub-sample volume [mL]	Components
250	HCO ₃ ⁻ , pH, Electric conductivity (EC)
125*	Na, K, Ca, Mg, Al, Fe, SO ₄ -S
250	Cl ⁻ , Br ⁻
500	³ H
100	δD, δ18O

* Filtered 0.40 μm, 1% HNO₃.

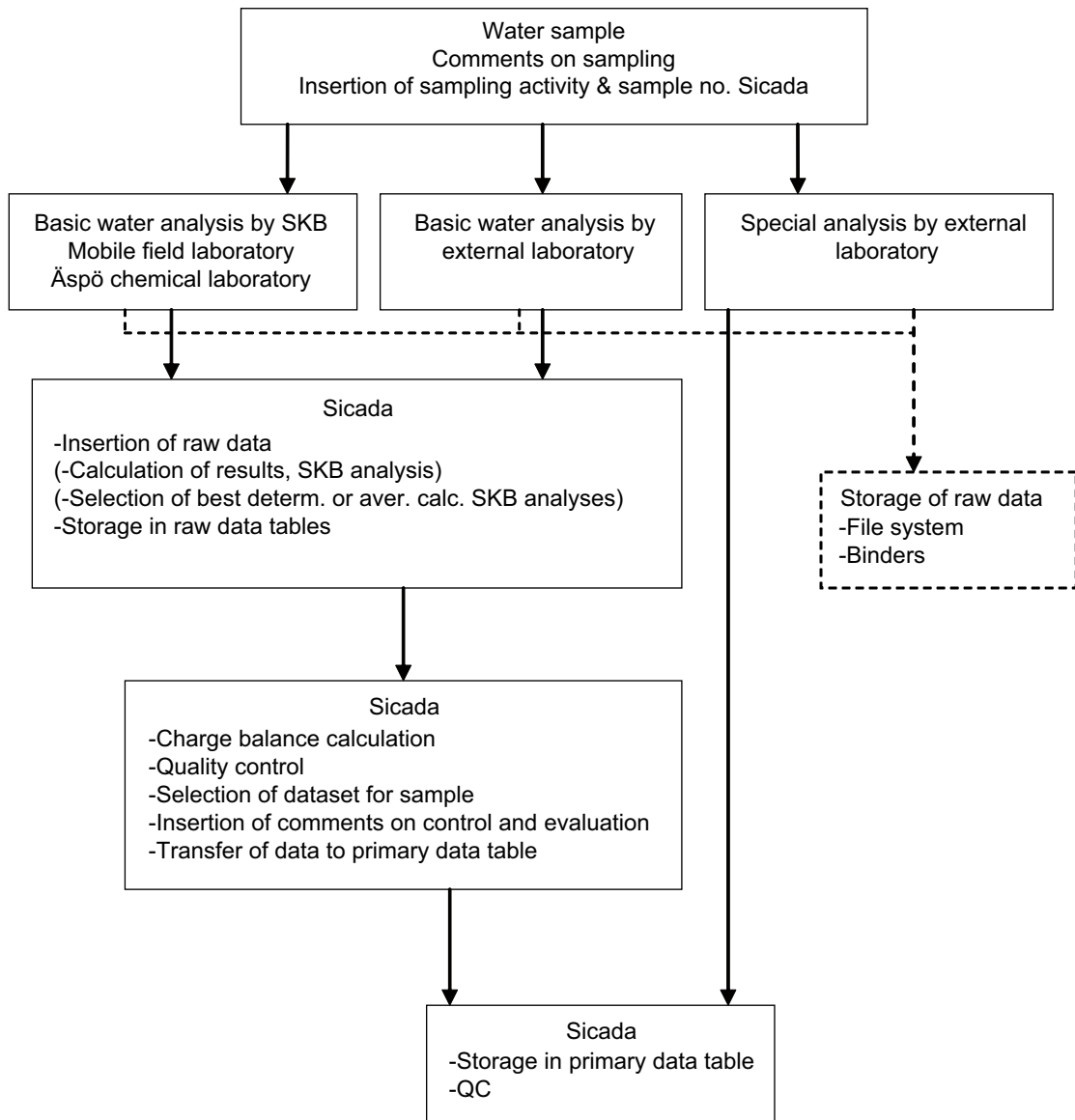


Figure 4-2. Overview of data management for hydrogeochemical data.

4.4 Nonconformities

By mistake, three samples lack analyses of aluminium since this was not ordered from the consulted laboratory.

5 Results

5.1 Basic water analyses

The basic water analyses include the major components Na, K, Ca, Mg, SO₄-S, Cl⁻, HCO₃⁻ and Br⁻. Furthermore, aluminium analyses and measurements of pH and electric conductivity (EC) were conducted. The basic water analysis data are compiled in Appendix 2, Table A2-1.

Calculations of the relative charge balance error may give an indication of the quality and uncertainty of the major constituents data also for precipitation. Normally, for surface waters, a relative charge balance error within $\pm 10\%$ is considered acceptable. However, the concentrations in precipitation samples are much lower and close to or below the reporting limit for many constituents. Therefore, analytical errors have a large impact on the charge balance and the precipitation samples often exceed this limit, see Figure 5-1.

5.2 Isotope analysis

The isotope determinations include the stable isotopes δD and $\delta^{18}O$ as well as the radioactive isotope ³H (Tritium). The isotope data are compiled in Appendix 2, Table A2-2.

Sampling for isotope determinations may be biased by evaporation during summer time.

The diagram for $\delta^{18}O$ (deviation from Standard Mean Ocean Water) versus δD (dev. SMOW) in Figure 5-2, corresponds well with the “Global meteoric water line” which is based on precipitation data from around the world /3/.

The variation of the tritium content in precipitation from Forsmark, July 2005– July 2007, is displayed in Figure 5-3. The contents in the few samples from Sjötorp are also shown and they follow the same trend.

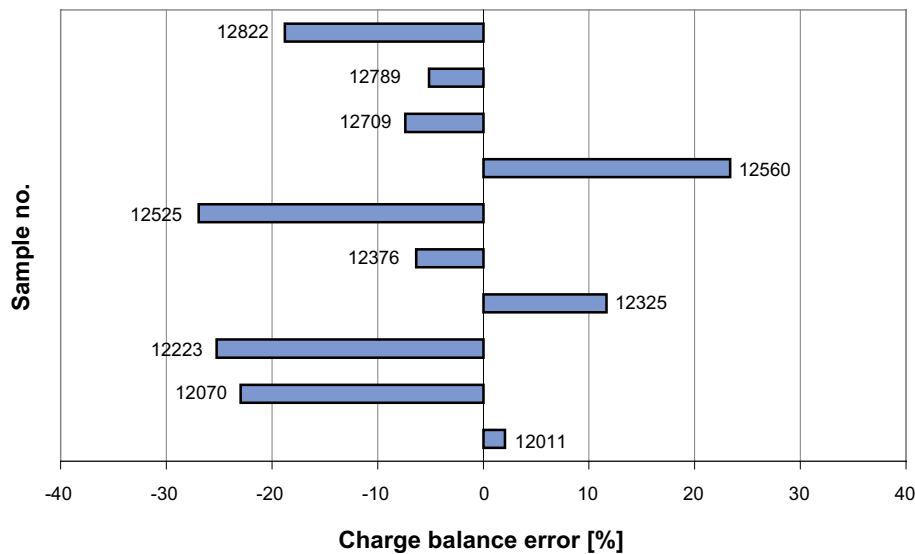


Figure 5-1. Calculated relative charge balance errors for the different precipitation samples.

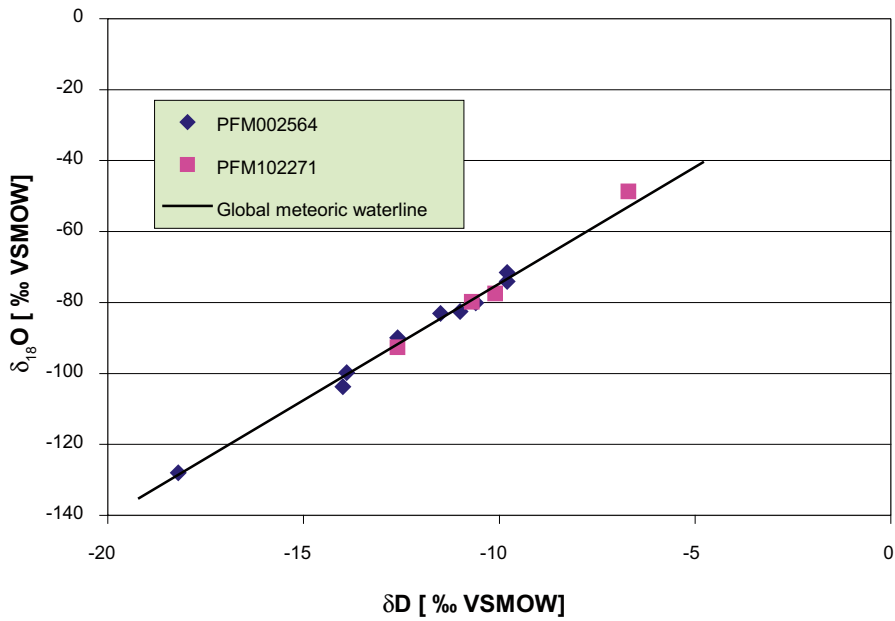


Figure 5-2. $\delta^{18}\text{O}$ plotted versus δD and compared with the “global meteoric water line”. PFM002564 = sampling location at the Forsmark site and PFM102271 = sampling location in Sjötorp.

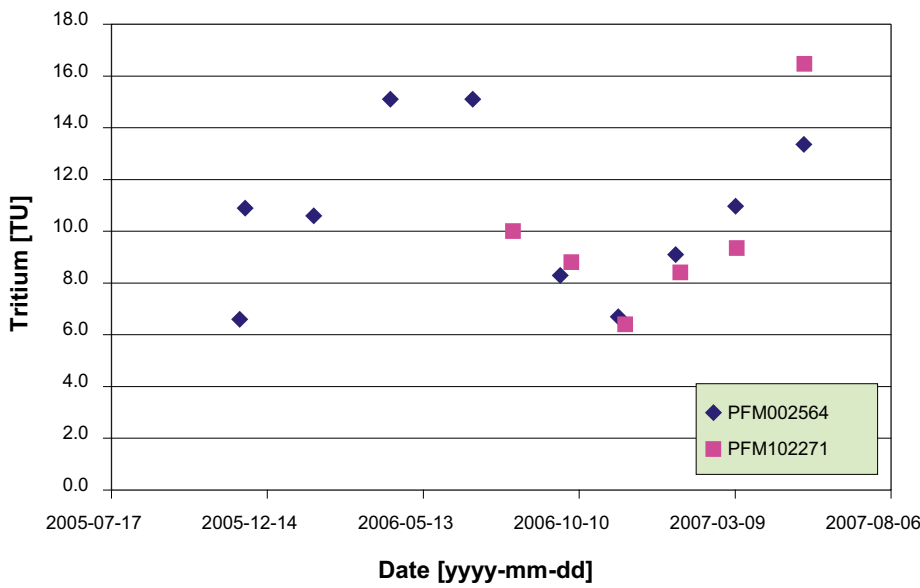


Figure 5-3. Tritium contents in the precipitation during the sampling period. The few tritium data from the reference point in Sjötorp is also given. PFM002564 = sampling location at the Forsmark site and PFM102271 = sampling location in Sjötorp.

6 Summary and discussions

This report documents the first one and a half year of precipitation sampling within the monitoring programme in Forsmark. The results from the sampling and analyses performed are summarised below:

- The Tritium results from precipitation in Forsmark and from the reference point in Sjötorp show very similar values even if the sampling periods do not agree completely.
- Aluminium contamination occurs at times. Especially sample no. 12822, the first sample collected with the new equipment, was affected by this deficit.
- The quality of the analytical data was considered reasonable, considering the very low concentrations. Analytical errors have a large impact on the relative charge balance errors and charge balance criteria are hardly useful for quality judgements for precipitation water, see section 5-1.

References

- /1/ **SKB, 2001.** Site investigations. Investigation methods and general execution programme. SKB R-01-29. Svensk Kärnbränslehantering AB.
- /2/ **Nilsson D, 2005.** Forsmark site investigation. Sampling and analysis of precipitation, years 2002 to 2005. SKB P-05-143. Svensk Kärnbränslehantering AB.
- /3/ **Craig H, 1961.** Isotopic variations in meteoric waters. Science 133, 1702–1703.

Sampling and analytical methods

Table A1-1. 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 (1 mL HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Fe(II), Fe(tot)	Fe(II), Fe(tot)	Plastic (Acid washed)	500	Yes	Yes (5 mL HCl)	Spectrophotometry Ferrozine method	As soon as possible the same day
Hydrogen sulphide	HS-	Glass (Winkler)	About 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 HNO ₃)	ICP-AES ICP-MS	Not critical (month)
Dissolved organic Carbon, dissolved inorganic Carbon	DOC, DIC	Plastic	250 25	Yes	Frozen, transported in isolated bag	UV oxidation, IR Carbon analysator Shimadzu TOC5000	Short transportation time
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	Not critical (month)
Chlorine-37	Chlorine-37	Plastic	100	No	–	MS	

Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/Conservation*	Analysis method	Analysis within – or delivery time to lab.
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	Nej	–	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)	Ar, N ₂ , CO ₂ , O ₂ , CH ₄ , H ₂ , CO, C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₈	Cylinder of stainless steel	200	No	No	GC	Immediate transport
Colloids	Filter series and fractionation (see below)	Polycarbonate filter	0.45, 0.2 and 0.05 µm	–	N ₂ atmosphere	ICP-AES ICP-MS	Immediate transport
Humic and fulvic acids	Fractionation	Fractions are collected in plastic bottles	250	–	N ₂ atmosphere	UV oxidation, IR (DOC)	Immediate transport
Archive samples with acid	–	Plast (washed in acid)	100×2 **	Yes	Yes (1 mL HNO ₃)	–	Storage in freeze container
Archive samples without acid	–	Plastic	250×2 **	Yes	No	–	Storage in freeze container
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 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
LSS	Liquid Scintillation Spectroscopy

Table A1-2. Reporting limits and measurement uncertainties

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
pH	Potentiometric	3–10	pH unit	± 0.1
EC	Electrical Conductivity meas.	1–150 150–10,000	mS/m	5% 3%
HCO ₃	Alkalinity titration	1	mg/L	4%
Cl ⁻	Mohr- titration	≥ 70	mg/L	5%
Cl ⁻	IC	0.5–70		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 ⁻	IC	DL 0.2, RL 0.5	mg/L	13%
F ⁻	Potentiometric	DL 0.1, RL 0.2		12%
I ⁻	ICP SFMS	0.001, 0.004, 0.010 ⁴	mg/L	25% ⁵
Na	ICP AES	0.1	mg/L	13%
K	ICP AES	0.4	mg/L	12%
Ca	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%
NO ₃ 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)
NH ₄ as N	Spectrophotometry, SKB	11	µg/L	30% (11–20 µg/L) 25% (20–50 µg/L) 12% (50–1,200 µg/L)
NH ₄ as N	Spectrophotometry external laboratory	0.8	µg/L	0.8 (0.8–20 µg/L) 5% (> 20 µg/L)
PO ₄ 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%

Component	Method ¹	Reporting limits (RL), detection limits (DL) or range ²	Unit	Measurement uncertainty ³
POC ⁷	/1/	1	µg/L	4%
Tot-N ⁷	/1/	10	µg/L	4%
Tot-P ⁷	/1/	0.5	µg/L	6%
Al,	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
Hg	ICP AFS	0.002	µg/L	10.7% ⁶
Co	ICP SFMS	0.005, 0.02, 0.05 ⁴	µg/L	25.9% ⁶
V	ICP SFMS	0.005, 0.03, 0.05 ⁴	µg/L	18.1% ⁶
Cu	ICP SFMS	0.1, 0.2, 0.5 ⁴	µg/L	14.4% ⁶
Ni	ICP SFMS	0.05, 0.2, 0.5 ⁴	µg/L	15.8% ⁶
P	ICP SFMS	1, 5, 40 ⁴	µg/L	16.3% ⁶
As	ICP SFMS	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
Tl	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%
δ ² H	MS	2	‰ SMOW ⁷	0.9 (one standard deviation)
δ ¹⁸ O	MS	0.1	‰ SMOW ⁷	0.1 (one standard dev.)
³ H	LSC	0.8	TU ⁸	0.8
δ ³⁷ Cl	A (MS)	0.2	‰ SMOC ¹⁰	0.2 ¹⁷
δ ¹³ C	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, ³⁰ 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: $pmC = 100 \times e^{((1.950 - y - 1.031)/6.274)}$
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: $\delta y\text{‰} = 1,000 \times (K_{\text{sample}} - K_{\text{standard}}) / K_{\text{standard}}$, where K= the isotope ratio and y = ²H, ¹⁸O, ³⁷Cl, ¹³C or ³⁴S etc.
- ¹⁷ SKB estimation from duplicate analyses by the contracted laboratory.

Appendix 2

Compilation of water analysis data

Table A2-1. Water Composition

Idcode		Sampling date and time	Sample no.	Al µg/L	Br mg/l	Ca mg/L	Cl- mg/L	EC_L mS/m	Fe mg/L	HCO3- mg/L	K mg/L	Mg mg/L	Na mg/L	pH_L	SO4_S mg/L
PFM002564	2005-11-17	2005-11-17	12011	–	< 0.2	0.42	0.952	2.10	< 0.02	<1	< 0.4	< 0.09	0.69	5.25	0.333
PFM002564	2005-11-22	2006-01-23	12070	–	< 0.2	0.49	0.719	1.61	< 0.02	<1	< 0.4	< 0.09	0.44	4.90	0.956
PFM002564	2006-01-27	2006-04-10	12223	0.037	< 0.2	0.19	0.639	4.08	0.037	<1	< 0.4	< 0.09	0.41	4.23	0.650
PFM002564	2006-04-11	2006-06-29	12325	< 0.06	< 0.2	0.68	0.300	1.56	< 0.02	1.5	0.76	0.100	0.63	5.66	0.567
PFM002564	2006-06-29	2006-09-20	12376	< 0.06	< 0.2	0.43	0.500	< 1	< 0.02	<1	< 0.4	< 0.09	0.28	5.40	0.417
PFM002564	2006-11-16	2007-01-10	12560	0.399	0.003	0.84	0.700	1.37	0.011	<1	< 0.4	< 0.09	0.40	4.68	0.190
PFM002564	2006-09-21	2006-11-15	12525	< 0.06	0.004	< 0.1	1.327	1.42	< 0.02	<1	< 0.4	< 0.09	0.44	4.77	0.319
PFM002564	2007-01-10	2007-03-01	12709	–	0.009	0.13	2.300	1.79	< 0.02	<1	< 0.4	0.167	1.24	4.84	0.277
PFM002564	2007-03-09	2007-05-10	12789	0.113	< 0.2	0.90	1.400	2.01	< 0.02	<1	0.57	0.178	0.89	5.40	1.080
PFM002564	2007-05-14	2007-06-26	12822	0.017	< 0.2	0.33	0.600	1.66	< 0.02	<1	< 0.4	< 0.09	0.28	4.62	0.527

< "value" = below reporting limit

RCB % = Rel. charge balance error %

SICADA: water_composition

Table A2-2. Isotopes (H- and O-isotopes)

Idcode		Sampling date	Sample no.	d2H dev SMOW	3H TU	d18O dev SMOW
PFM002564	2005-11-17	2005-11-17	12011	-83.1	6.6	-11.50
PFM002564	2005-11-22	2006-01-23	12070	-128.0	10.9	-18.20
PFM002564	2006-01-27	2006-04-10	12223	-89.9	10.6	-12.60
PFM002564	2006-04-11	2006-06-29	12325	-71.5	15.1	-9.80
PFM002564	2006-06-29	2006-09-20	12376	-80.1	15.1	-10.60
PFM002564	2006-09-21	2006-11-15	12525	-99.8	8.3	-13.90
PFM002564	2006-11-16	2007-01-10	12560	-82.5	6.7	-11.00
PFM002564	2007-01-10	2007-03-01	12709	-103.7	9.1	-14.00
PFM002564	2007-03-09	2007-05-10	12789	-74.1	11.0	-9.80
PFM002564	2007-05-14	2007-06-26	12822	-47.3	13.4	-7.2
PFM102271	2006-08-07	2006-10-02	12062	-48.7	10.0	-6.7
PFM102271	2006-10-02	2006-11-23	12526	-	8.8	-
PFM102271	2006-11-23	2007-01-15	12588	-79.8	6.4	-10.7
PFM102271	2007-01-15	2007-03-10	12741	-92.6	8.4	-12.6
PFM102271	2007-03-10	2007-05-14	12793	-77.5	9.4	-10.1
PFM102271	2007-05-14	2007-06-26	12823	-	16.5	-

A: Results to be reported

SICADA: isotopes_1