P-05-89

Oskarshamn site investigation

Hydrochemical logging in KLX03

Results from isotope determinations (^{3}H, δD and δ^{18}O)

Cecilia Berg, Geosigma AB

June 2005

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1651-4416
SKB P-05-89

Oskarshamn site investigation

Hydrochemical logging in KLX03

Results from isotope determinations (^{3}H, δD and δ^{18}O)

Cecilia Berg, Geosigma AB

June 2005

Keywords: Core drilled borehole, Groundwater, Water sampling, Chemical analyses.

Abstract

Hydrochemical logging or so called tube sampling has been performed in the core drilled borehole KLX03. The method is a fast and simple sampling technique to obtain information of the chemical composition of the water along an open borehole. The equipment consists of an approximately 1,000 metres long polyamide tube divided into units of 50 metres.

The water content in each tube unit constituted one sample. Every other sample, starting with the uppermost unit, was analysed according to SKB chemistry class 3 (excluding isotope options). The performance and results from this sampling has been reported in a previous report /1/. The following report gives the results from the performed isotope determinations of tritium (^{3}H), deuterium (δD) and $\delta^{18}O$. Samples for isotope determinations were collected at the sampling occasion and stored in a freezer (tritium in a refrigerator) for approximately two months before they were sent to the consulted laboratories for analyses.

Sammanfattning

Hydrokemisk loggning, även kallad slangprovtagning, har utförts i kärnborrhålet KLX03. Hydrokemisk loggning är en snabb och enkel provtagningsteknik för att erhålla information om vattenpelarens kemiska sammansättning längs ett öppet borrhål. Utrustningen utgörs av en cirka 1 000 meter lång polyamid slang uppdelad i enheter om vardera 50 meter.

Innehållet i en slangenhet utgör ett prov. Varannan enhet, med start från den översta, analyserades i enlighet med SKB kemiklass 3 utan tillägg i direkt anslutning till provtagningstillfället. Utförande och resultat från denna provtagning har rapporterats i en tidigare primärdatarapport /1/. Denna rapport redovisar resultaten från utförda isotopanalyser av tritium (^{3}H), deuterium (δD) och $\delta^{18}O$. Isotopprover togs ut i samband med provtagningen och sparades i frys respektive kyl (tritium) i cirka två månader innan de sändes iväg för analys till de konsulterade laboratorierna.

Contents

1 Introduction

This document reports isotope results from the Hydrochemical logging in borehole KLX03, which is one of the activities performed within the site investigation at Oskarshamn /2/. The work was carried out in accordance with activity plan SKB AP PS 400-04-079. In Table 1-1 controlling documents for performance of this activity are listed. Both activity plan and method descriptions are SKB's internal controlling documents.

This report is a complement to the previous report regarding the Hydrochemical logging in KLX03 /1/, which documented the performance and results from analyses of major constituents, anions, flushing water content, electric conductivity, pH and hydrogen carbonate. The data from the activity is reported to the database SICADA.

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

Activity plan	**Number**	**Version**
Hydrokemisk loggning i KLX03	AP PS 400-04-079	1.0
Method descriptions	**Number**	**Version**
Metodbeskrivning för hydrokemisk loggning	SKB MD 422.001	1.0

2 Objective and scope

Hydrochemical logging was performed in order to obtain an overview of the chemical composition of the water along the open borehole KLX03. The technique used for sampling is fast and simple even at great depth.

The analysis program has previous been carried out according to SKB chemistry class 3 without isotope options and reported in a previous report /1/. The isotopes reported in this report were sent to be analysed approximately two months after the sampling occasion i.e. at the end of November. Until they were sent for analyses they were stored in a freezer (tritium in a refrigerator). The conducted isotope determinations include tritium, $\delta^{18}O$ and deuterium.

3 Performance

3.1 Hydrochemical logging

The hydrochemical logging in KLX03 was performed September 21, 2004, according to the controlling documents for the activity (see Table 1-1).

The performance of the activity is described in a previous report regarding the hydrochemical logging in KLX03 /1/.

3.2 Sample treatment and chemical analysis

An overview of sample treatment and analysis routines is given in Appendix 1.

An overview showing the samples obtained at the logging occasion is given in Table 3-1. The sample portions for isotope analyses were stored in a freezer at SKB (tritium in a refrigerator) at the time of the hydrochemical logging. Samples collected for determination of tritium, $\delta^{18}O$ and deuterium were analysed at the consulted laboratories approximately two months after the sampling performance. Remaining isotope samples collected are still stored in a freezer. The data from the hydrochemical logging are stored in the database SICADA. The SKB sample numbers are 7778 to 7797.

Due to the lack of water in the first tube unit, archive samples from the second tube unit was not obtained. Water intended for archive samples in the second unit were used to fill sample bottles for analyses of anions, $\delta^{2}H$ and $\delta^{18}O$, $\delta^{37}Cl$, $^{10}B/^{11}B$ from the first section (0–40 m).

Table 3-1. Overview of samples collected at the hydrochemical logging in KLX03. Filled cells represent collected samples. Dark (blue) filling represents samples reported in a previous report, light (yellow) filling represents isotope samples that has been analysed, dashed yellow filling represents samples stored in freezer (carbon isotopes in a refrigerator) and dashed (purple) cells represent archive samples.

Sample information			Collected sample portions											Archive
Tube unit	Length (m)	SKB no	Cond, pH, alk	Major Comp	Uranine	Anions	^{3}H	δD δ^{18}O	δ^{37}Cl	^{10}B	^{87}Sr	δ^{34}S	Carbon isotopes	Filtered 2×250 mL
1	0	7778						ω	ж	ж				
	40													
2		7779												
	90													
3		7780												
	140													
4		7781												
	190													
5		7782												
	240													
6		7783												
	290													
7		7784												
	340													
8		7785												
	390													
9		7786												
	440													
10		7787												
	490													
11		7788												
	540													
12		7789												
	590													
13		7790												
	640													
14		7791												
	690													
15		7792												
	740													
16		7793												
	790													
17		7794												
	840													
18		7795												
	890													
19		7796												
	940													
20		7797												
	990													

ж filled with sample water from tube unit two.
ω partly filled with sample water from tube unit two.

3.3 Data handling

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

Several 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 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 ±5% are considered acceptable (in surface waters ±10%).

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

- 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 3-1.

3.4 Nonconformities

The activity was performed without any deviations from the controlling documents.

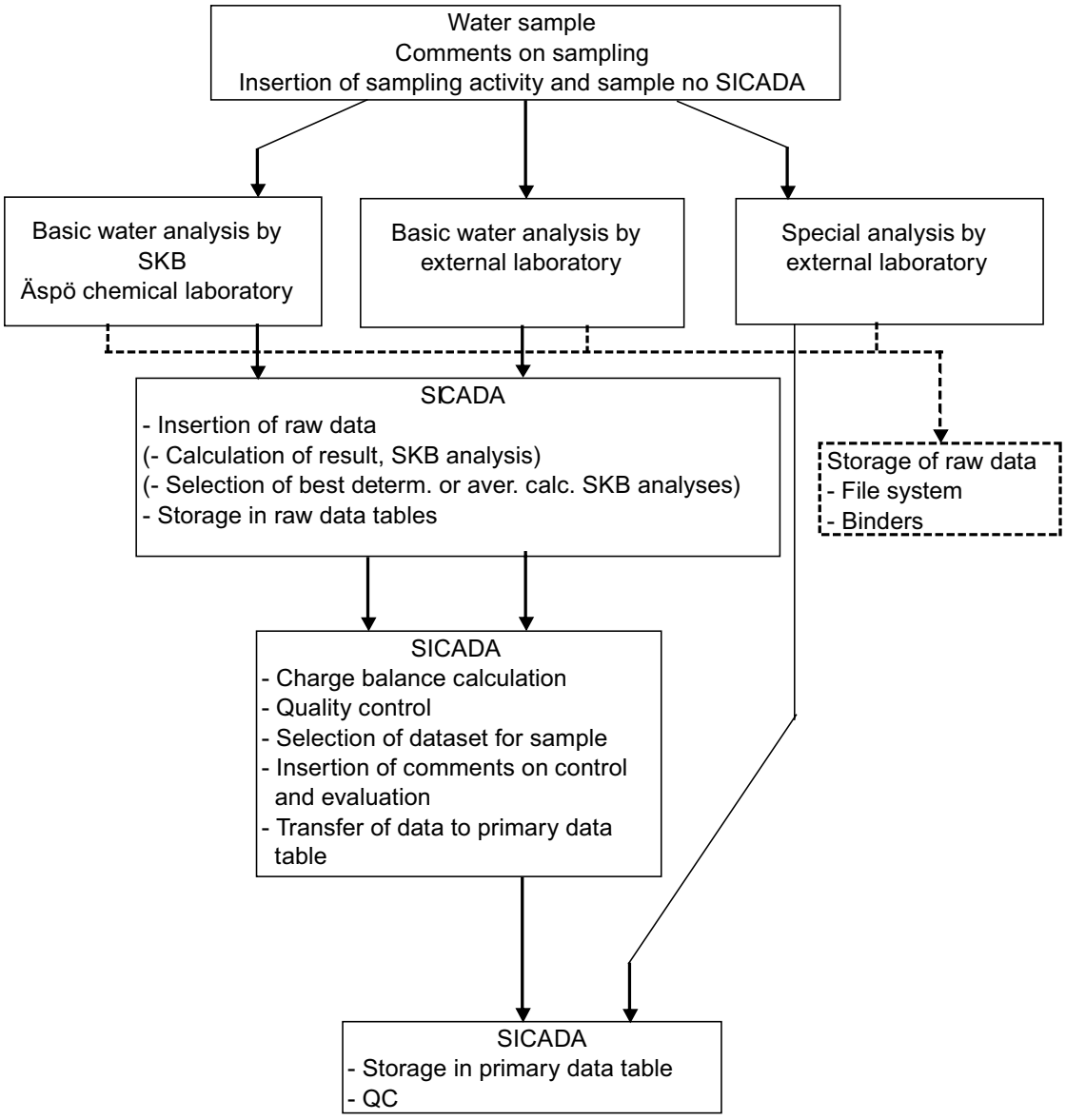

Figure 3-1. *Overview of data management for hydrogeochemical data. This report only handles the "Special analyses by external laboratory". (The basic water analyses are reported in a previous report /1/).*

4 Results

4.1 Analysis results

The results from the conducted isotope determinations are given in Appendix 2. Diagrams showing the tritium and $\delta^{18}O$ values along the borehole received from the hydrochemical logging are presented in Figure 4-1. Results from deuterium determinations are shown in Table 4-1. Results are plotted for the mid-length of each tube unit, for example the first tube is plotted at 20 metres.

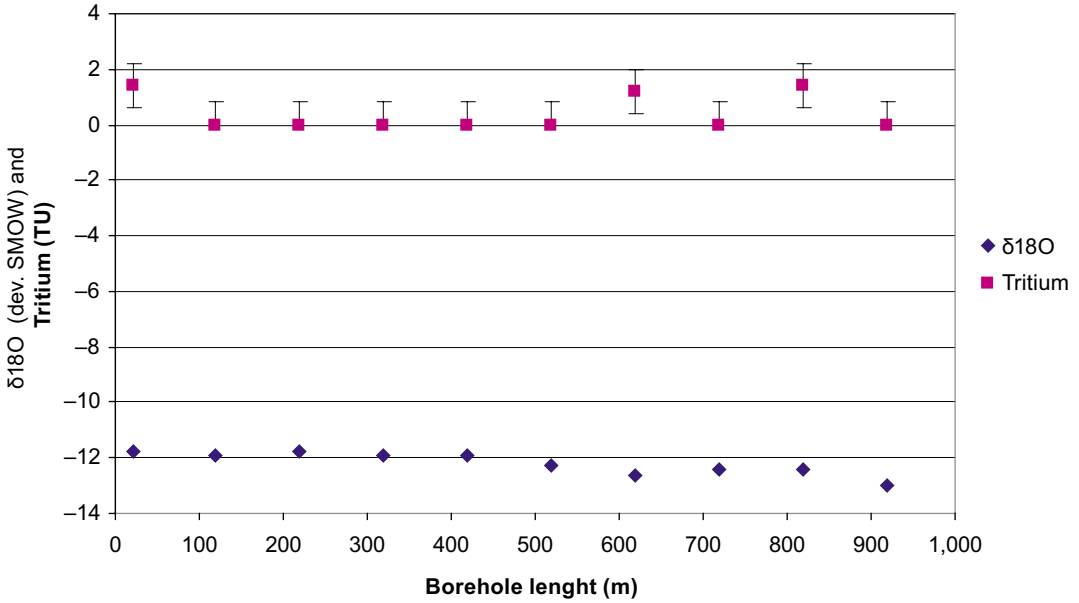

Figure 4-1. *Tritium and $\delta^{18}O$ data from samples collected in the core drilled borehole KLX03 at the hydrochemical logging.*

Table 4-1. Deuterium determinations for samples collected at the hydrochemical logging in KLX03.

Sample SKB no	δD (dev SMOW)
7778	–83.6
7780	–84.5
7782	–83.7
7784	–84.6
7786	–84.5
7788	–89.4
7790	–90.5
7792	–87.2
7794	–90.5
7796	–95.8

5 References

/1/ **Berg C, Wacker P, 2004.** Oskarshamn site investigation. Hydrochemical logging in KLX03A. SKB P-04-299, Svensk Kärnbränslehantering AB.

/2/ **SKB, 2001.** Generellt genomförande program för platsundersökningar. SKB R 01-10, Svensk Kärnbränslehantering AB.

Appendix 1

Sampling and analysis methods

Table A1-1. Overview of general sample handling routines and analysis methods.

Component group	Component/element	Sample container (material)	Volume (mL)	Filtering	Preparation/conservation*	Analysis method	Laboratory***	Analysis within – or delivery time to lab
Anions 1	HCO_3 pH(lab) cond (lab)	Plastic	250	No	No	Titration Pot meas, Cond meas	Äspö's chemistry lab	The same day – maximum 24 hours
Anions 2	Cl, SO_4, Br^-, F^-, I^-	Plastic	250	Yes (not in the field)	No	Titration (Cl^-) IC (Cl^-, SO4, Br^-, F^-) ISE (F^-)	Äspö's chemistry lab	Not critical (month)
Cations, Si and S according to SKB class 3	Na, K, Ca, Mg, S(tot), Si(tot), Li, Sr	Plastic (at low conc acid washed bottles)	100	Yes (not in the field)	Yes (not in the field, 1 mL HNO_3)	ICP-AES ICP-MS	Analytica AB	Not critical (month)
Environmental isotopes	^2H, ^{18}O	Plastic	100	No	– –	MS	IFE	Not critical (month)
Tritium,	^3H (enhanced)	Plastic (dry bottle)	500	No	–	LSC	Univ Of Waterloo	Not critical (month)
Chlorine-37	Chlorine-37	Plastic	500	No	–	ICP MS	Univ Of Waterloo	Not critical (month)
Carbon isotopes	^{13}C, ^{14}C	Glass (brown)	100×2	No	–	(A)MS	Univ Of Waterloo The Ångström laboratory, Uppsala	A few days
Sulphur isotopes	^{34}S	Plastic	500–1,000	No	–	Combustion, ICP MS	IFE	No limit
Strontium-isotopes	$^{87}Sr/^{86}Sr$	Plastic	100	No	–	TIMS	IFE	Days or Week
Boron isotopes	^{10}B	Plastic	100	Yes	Yes (1 mL HNO_3)	ICP – MS	Analytica AB	No limit
Archive samples without acid	–	Plastic	250×2**	Yes	No	–	–	Storage in freeze

* Suprapur acid is used for conservation of samples.
** Minimum number, the number of archive samples can vary depending on how many similar samples that are collected at the same occasion.
*** Full name and address is given in Table A1-2.

Abbreviations and definitions:

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

Table A1-2. Consulted laboratories, full name and address.

Äspö waterchemical laboratory (SKB)
Analytica AB Aurorum 10 977 75 Luleå (Nytorpsvägen 16 Box 511 183 25 Täby)
Environmental Isotope Laboratory Dep Of Earth Sciences University of Waterloo Waterloo, Ontario N2L 3G1 CANADA
Institutt for energiteknik (IFE) Insituttveien 18 P O Box 40 2027 Kjeller NORGE
The Ångström laboratory Box 534 SE-751 21 Uppsala

Appendix 2

Isotopes, compilation of H-, and O-isotopes

Compilation May 2005

Idcode	Secup	Seclow	Sample	δD	^{3}H	δ^{18}O	δ^{37}Cl	^{10}B/^{11}B	^{87}Sr/^{86}Sr	δ^{34}S	δ^{13}C	^{14}C
	m	m	no	dev SMOW	TU	dev SMOW	dev SMOC	no unit	no unit	dev CDT	dev PDB	pmC
KLX03	0	40	7778	–83,6	1,4	–11,8	xxx	xxx	–	–	–	–
KLX03	40	90	7779	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	90	140	7780	–84,5	<0.8	–11,9	xxx	xxx	xxx	–	–	–
KLX03	140	190	7781	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	190	240	7782	–83,7	<0.8	–11,8	xxx	xxx	xxx	–	–	–
KLX03	240	290	7783	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	290	340	7784	–84,6	<0.8	–11,9	xxx	xxx	xxx	–	–	–
KLX03	340	390	7785	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	390	440	7786	–84,5	<0.8	–11,9	xxx	xxx	xxx	–	–	–
KLX03	440	490	7787	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	490	540	7788	–89,4	<0.8	–12,3	xxx	xxx	xxx	–	–	–
KLX03	540	590	7789	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	590	640	7790	–90,5	1,2	–12,6	xxx	xxx	xxx	–	–	–
KLX03	640	690	7791	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	690	740	7792	–87,2	<0.8	–12,4	xxx	xxx	xxx	–	–	–
KLX03	740	790	7793	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	790	840	7794	–90,5	1,4	–12,4	xxx	xxx	xxx	–	–	–
KLX03	840	890	7795	–	–	–	–	–	–	xxx	xxx	xxx
KLX03	890	940	7796	–95,8	<0.8	–13,0	xxx	xxx	xxx	–	–	–
KLX03	940	990	7797	–	–	–	–	–	–	xxx	xxx	xxx

– = Not analysed
A = results will be reported later
x = No result due to sampling problems
xx = No result due to analytical problems
xxx = Stored in a freezer
< “value” = result below detection limit