P-09-45

Site investigation SFR

Presentation and evaluation of hydrogeochemical data from SFR-boreholes, 1984–2007

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August 2009

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Data in SKB's database can be changed for different reasons. Minor changes in SKB's database will not necessarily result in a revised report. Data revisions may also be presented as supplements, available at www.skb.se.

Contents

1 Introduction

The Swedish Nuclear Fuel and Waste Management Company (SKB) is undertaking geoscientific investigations in the Forsmark area, adjacent to the SFR underground repository, located about 150 km north of Stockholm. The investigations are being carried out to meet the planned expansion of the SFR facility for low and medium active radioactive waste. The repository came into use in April 1988 and, at present, the stored waste volume is about 30,000 m^3 (total capacity is 63,000 m^3), consisting of operational waste from the Swedish nuclear power plants and radioactive waste from hospitals. The purpose of the ongoing investigations is to define and characterise a bedrock volume large enough to allow further storage of operational waste from Swedish nuclear power plants and future waste from the decommissioning and dismantling of nuclear power plant reactors /1/. Of several alternatives, an initial location will be investigated southwest of the present SFR tunnel system, see Figure 1-1.

This document presents an evaluation of existing hydrogeochemical data from 1984–2007, which represents one of the activities performed within the site investigation at SFR. The work was carried out in accordance with activity plan AP SFR-08-023, and the controlling documents for performing this activity are listed in Table 1-1. Both the activity plan and method descriptions are SKB's internal controlling documents.

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

Activity plan	Number	Version
Platsmodellering, Hydrogeochemistry version 0.1.	AP SFR-08-023	0.1
Method descriptions	**Number**	**Version**
Hantering av data och modeller inom Projekt SFR-utbyggnad – delprojekt undersökningar.	SKB MD SDU-103	0.1
Hantering av primärdata vid platsundersökningar.	SKB MD SDK-508	3.0

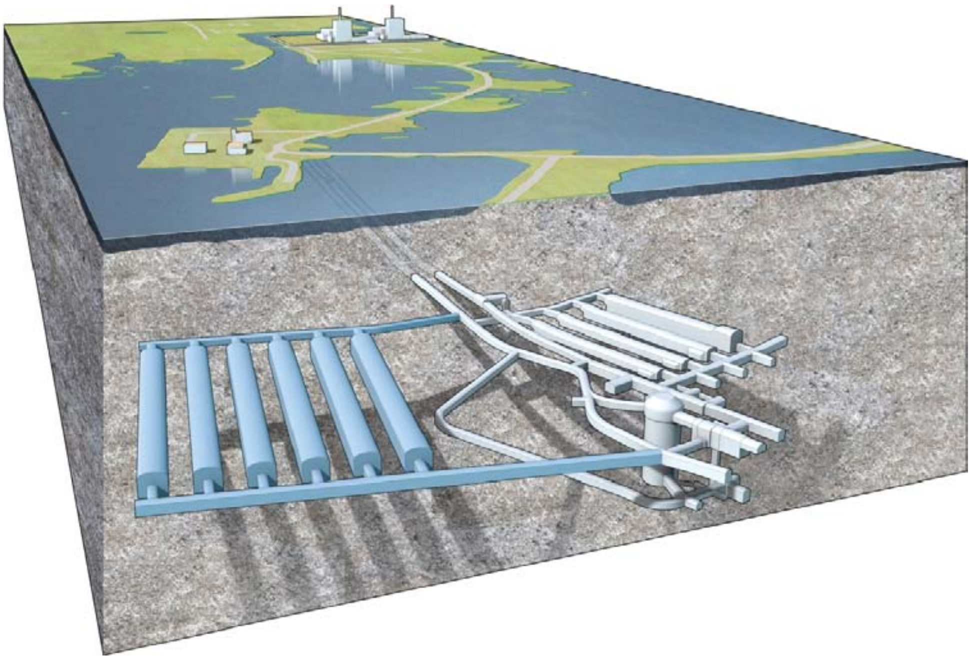

Figure 1-1. *One of several lay out proposals for the extension of the SFR-repository. The present SFR-repository is located to the right (light blue colour) while the planned new tunnel system is shown to the left (darker blue colour).*

Hydrogeochemical characterisation of groundwaters in boreholes drilled from the ground surface and from the construction tunnel in the present SFR facility, forms part of the ongoing geoscientific investigation work. However, there already exist hydrogeochemical data from the Forsmark region as a whole, which will comprise a substantial part of the data volume to be used for evaluation and modelling purposes. Available data from earlier hydrogeochemical investigations in boreholes in the SFR will constitute very important complementary information since the ongoing investigations include a relatively limited number of boreholes. Data from the recently completed site investigations in Forsmark (PLU) to locate a deep repository for spent nuclear fuel /2/ will also contribute to the understanding of the groundwater conditions in the SFR model area (SFR site), see Figure 1-2. Early data from SFR investigations during the construction phase of the existing SFR tunnel system (1984–1987), together with data from the routine SFR groundwater control or monitoring programme that has been ongoing since 1989, have been documented previously in several reports, see /3, 4, 5/ and /6/. The aim of the present report is to give an updated description and evaluation of these hydrogeochemical data based on recent experience gained from the PLU investigations. A systematic evaluation of the dataset will provide the basis to continued quantitative and qualitative hydrogeochemical modelling and interpretation work.

1.1 Model versions and content

An evaluation of the groundwater conditions at SFR, mainly concerning long term changes and trends due to open tunnel conditions, was reported in 2003 /6/. Although this modelling exercise did not result in a complete hydrochemical site description, it is the most recent work done, and therefore it constitutes the hydrogeochemical model version 0.0 for the planned modelling activities within the Project SFR extension. Model version 0.0 does not consider recent knowledge and experience obtained from the PLU investigations.

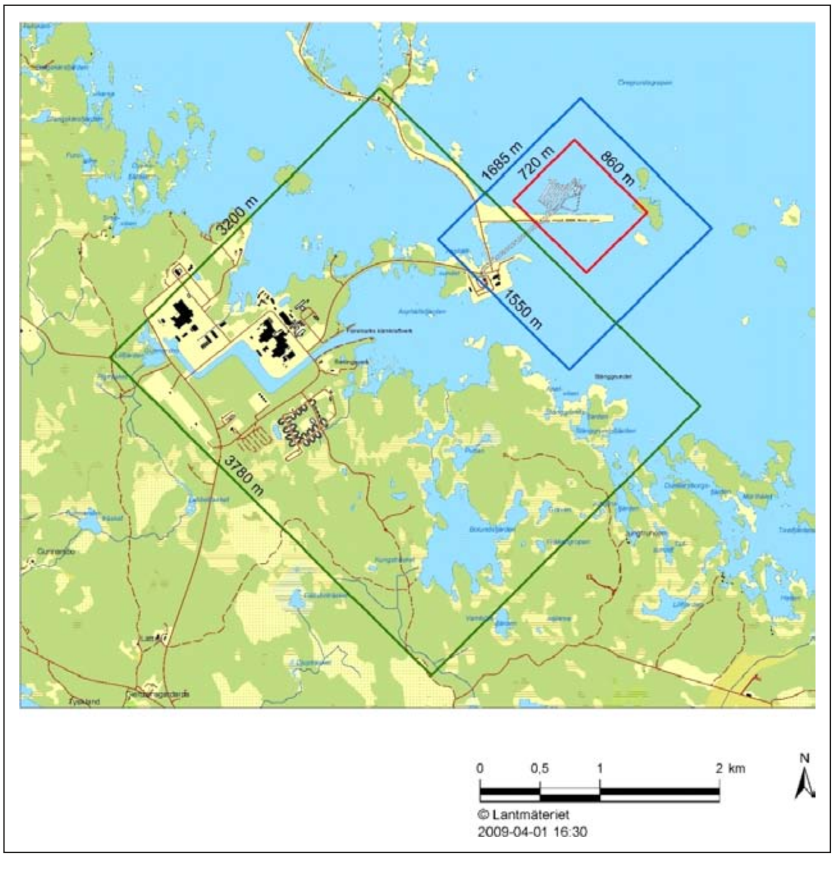

***Figure 1-2.** Regional (blue) and local (red) model domains for SFR model v. 0.1, in relation to the local model area of the Forsmark Site Investigation, model v. 2.2 (green).*

The modelling work for the SFR site will be performed in three steps resulting in three model versions (0.1, 0.2 and 1.0) from the modelling disciplines hydrogeology and hydrogeochemistry. The geology discipline will exclude version 0.2 and start producing model version 1.0 directly after version 0.1. Each of the modelling disciplines will iteratively exchange feedback during the sequential step by step development of model versions, not only to improve and/or reinforce the characterisation of the hydrogeologic system but also to achieve consistency in the development of the interdisciplinary conceptual models. Model versions 1.0 from each discipline will be documented in background reports prior to being finally integrated into the SFR Site Descriptive Model version 1.0. The content of each hydrogeochemical model version/report is presented in Table 1-2.

1.2 Scope of hydrogeochemistry model SFR v.0.1

This P-report (hydrogeochemical model version 0.1) describes and discusses available groundwater data from boreholes in the present SFR facility but does not present any proper hydrogeochemical model in the strict sense. In fact, version 0.1 treats mainly the same dataset as the preceding version 0.0. Therefore, mixing (M3) and mass balance calculations are not repeated. Besides the report, the complete dataset is compiled into a suitable format (SFR Hydrogeochemistry Table version 0.1) for continued modelling and stored in SKBDoc (database for modelling purposes). The dataset have been evaluated systematically with respect to quality and representativity and an assignment (categorisation) is made with respect to the value for further hydrogeochemical interpretation work. The data are presented in different plots, i.e. time series plots, x/y scatter plots and depth trend plots, as well as in 3D visualisations. This is done in order to identify different groundwater types, to describe their spatial distribution, and to reveal questionable data. Furthermore, with background information on relevant groundwater types from /6/ and /7/, a simple grouping is made based on chloride and magnesium concentrations and $\delta^{18}O$ ratios. The three groups encountered are groundwaters: 1) with a strong marine signature, 2) representing intermediate mixtures *(between 1 and 3),* and 3) with a significant glacial component.

Table 1-2. Hydrogeochemical model versions and contents.

Model version	Content	Date
0.1 (P-report)	Compilation of dataset including groundwater data from boreholes in the present SFR-facility (SFR Hydrogeochemistry Table version 0.1). Description and evaluation of the hydrochemical dataset and categorisation of groundwater samples according to their value for future modelling and interpretation work.	2009-08-31
0.2 (R-report)	Compilation of a dataset to include v 0.1 data as well as ground-water data from boreholes HFR101, HFR105, KFR101 and KFR102A (SFR Hydrogeochemistry Table version 0.2). Explorative analyses and M3 modelling. Constructing a preliminary hydrogeochemical model to include an adapted and detailed conceptual model for the SFR site regarding groundwater history and evolution. This will be based on the present PLU conceptual model for the Forsmark site.	2009-12-30
1.0 (R-report)	Compilation of a dataset to include v 0.2 data as well as groundwater data from boreholes HFR106, KFR105 and KFR106 (SFR Hydrogeochemistry Table version 1.0). Explorative analyses, M3 modelling and mass balance calculations. Final hydrogeochemical model including an adapted and detailed conceptual model for the SFR site regarding groundwater history and evolution, based on the present PLU conceptual model for the Forsmark site.	2010-08-31

2 Background

2.1 Geological and hydrogeological setting

Updates of the geological and hydrogeological models for the SFR site are presented in the corresponding geological and hydrogeological model version 0.1 reports, Curtis P et al. /8/ and Öhman J et al. /9/, respectively. The SFR area is situated within a high-strain belt that forms the north-easterly margin to the so-called Forsmark tectonic lens. The strongly deformed rocks consist of a heterogeneous package of mainly felsic to intermediate metavolcanic rocks intercalated with biotite-bearing metagranite /8/. Locally, these rocks have been intruded by considerable amounts of younger, often pegmatitic granite, see Figure 2-1. The modelled deformation zones in the local area are displayed in Figure 2-2 and appear simplified in Figure 2-3. Two regional vertical to steeply dipping zones ZFMWNW0001 (Singö) and ZFMNW0805A (zone 8) form the general SW and NW boundaries of the investigation area. Other steeply dipping deformation zones in the local volume and intersected by early boreholes are ZFMNE0870A and ZFMNE0870B (previously zone 9), ZFMNNW1209 (zone 6) and ZFMNNE0869 (zone 3). A single gently dipping deformation zone of importance for the hydrogeochemical conditions, ZFM871 (zone H2), is located just beneath the silo at SFR and covers most of the local model area.

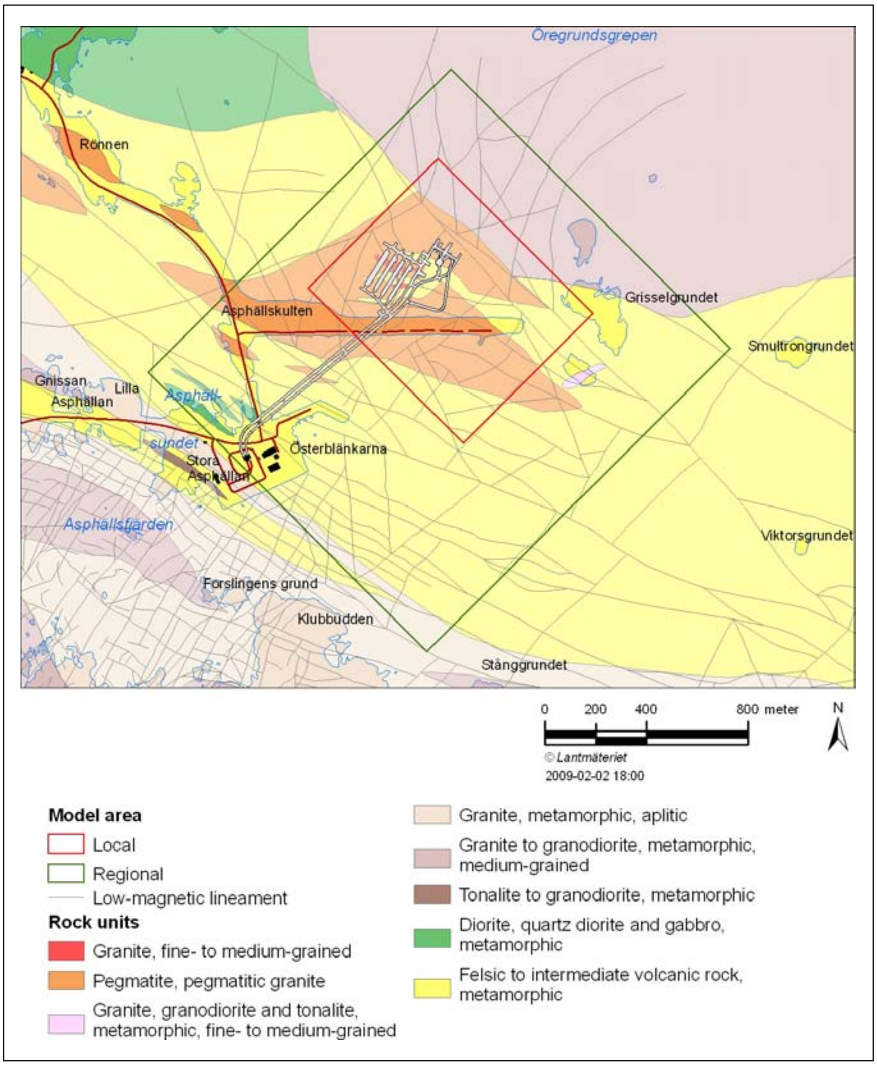

Figure 2-1. Bedrock geological map of the area around SFR with the local and regional SFR model areas included /8/.

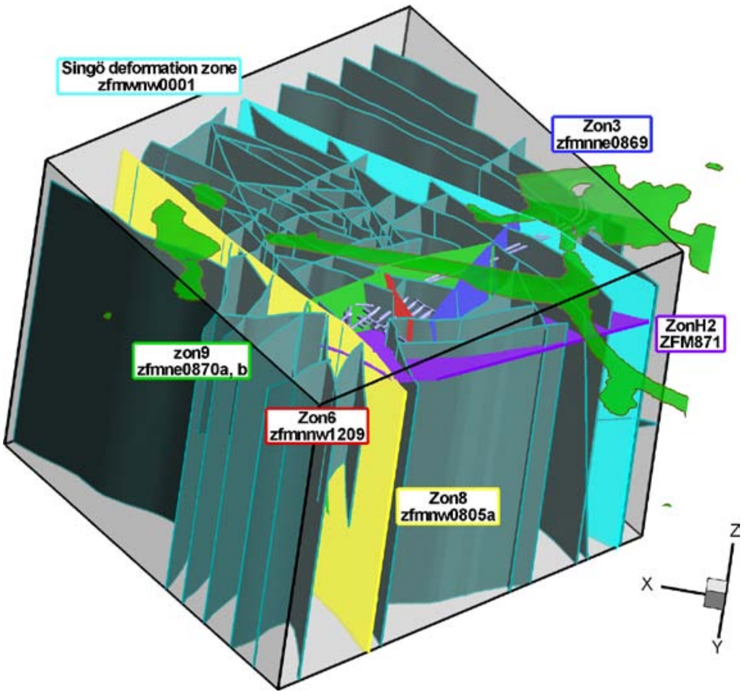

Figure 2-2. *Deformation zones of the regional SFR model volume as defined in the updated structural model SFR v. 0.1 /8/.*

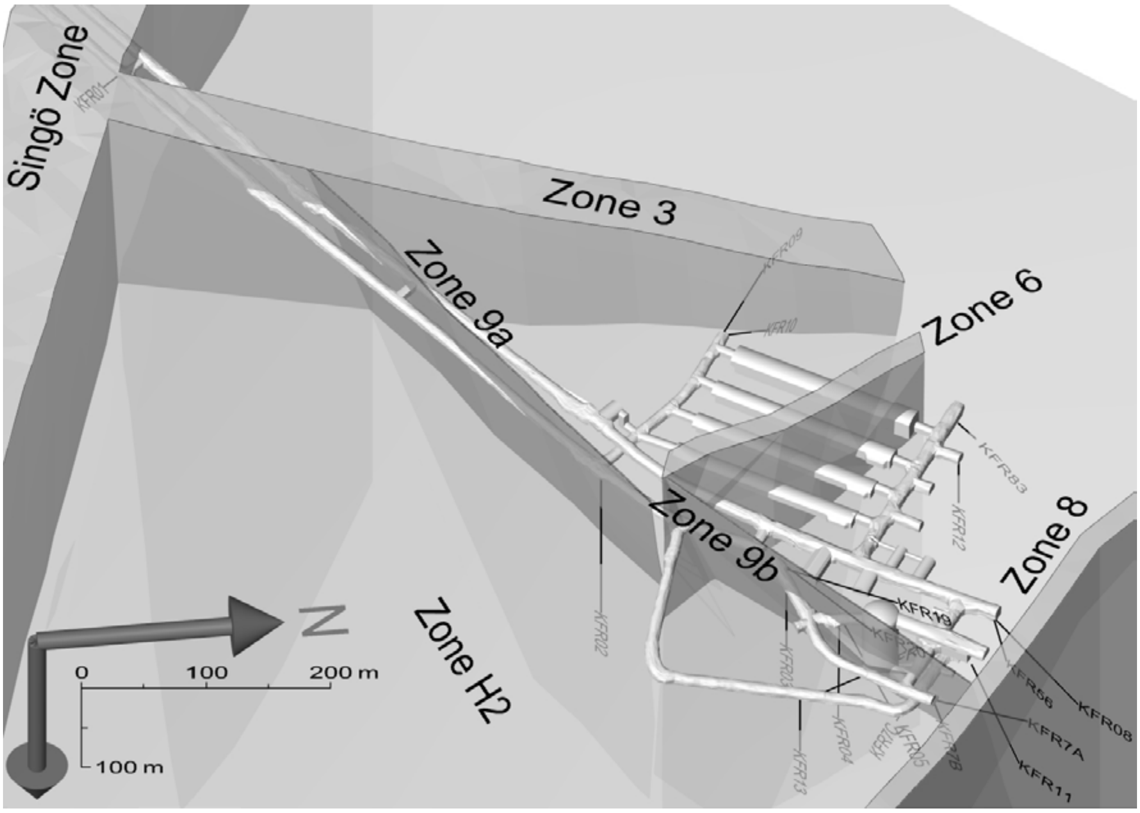

Figure 2-3. *3D presentation (no perspective distortion of size) of today's tunnel system in SFR showing the location of the deformation zones and boreholes. The zones are marked according to the SFR terminology. Zone names according to the system established during the Forsmark site investigation are as follows: Singö zone = ZFMWNW0001, Zone H2 = ZFM871, Zone 3 = ZFMNNE0869, Zone 6 = ZFMNNW1209, Zone 8 = ZFMNW0805A, Zone 9a = ZFMNE0870A, Zone 9b = ZFMNE0870B.*

2.2 Boreholes and borehole installations

About 20 years ago, packer systems were installed in most of the boreholes drilled from the present SFR tunnel system. Twelve of these old installations have been renewed during 2007/2008 due to the SFR expansion project but with the ambition to keep the section length distribution unchanged. Observations resulting from these replacements are listed in Table 2-1. The original packed-off sections in each borehole are given in Table 2-2. The precise positioning of these packer systems in the boreholes has been questioned. One reason for this is the uncertainty regarding the starting point that was used for the borehole length information; was it a point on the casing, or was it the tunnel wall surface close to the borehole orifice? However, according to subsequent checks of pipe lengths in dismantled old borehole equipment, the lengths given in Table 2-2 are correct to within 3 dm. The borehole lengths were found to be measured from the rock wall except for boreholes drilled into the tunnel floor. Here, the casing ('Top Of Casing' or 'TOC') was used as the starting point.

With respect to uncertainties in packer positions, there are other factors to consider when evaluating hydrochemical data from the SFR-boreholes drilled during the eighties:

- The original pipes were made of aluminium or ordinary iron and not of stainless steal as today. Consequently, when the old borehole installations were being replaced recently, severe corrosion was observed in both cases according to SKB internal documentation (Jönsson S, 2008. Installation och driftsättning av ny utrustning för grundvattenmonitering i 12 borrhål i SFR).
- Casings were made of ordinary iron and not of stainless steal.
- Leakage problems due to corroded equipment was observed in borehole KFR7A, see Table 2-1.
- Groundwater drawdown caused by the tunnel system has, with the passing of time, decreased the number of borehole sections possible to sample. Clogging by precipitates or bacteria are other reasons for decreased groundwater flow and sampling difficulties.

The hydrogeochemical data discussed in this report have all been obtained by sampling in boreholes with the original installations.

Table 2-1. Observations from replacement borehole equipment in SFR-boreholes (2007/2008).

Idcode:section	Observation	Probable reason
KFR05:3	Flow rate increased by a factor of 15 following replacement of the old packer equipment.	Clogging of pipes in the old equipment.
KFR19:1	The previously observed pressure decrease with the old equipment was normalised following replacement. Flow rate increased from zero to 0.36 mL/min after replacement.	Clogging of pipes in the old equipment.
KFR19:2	Flow rate increased from zero to 0.50 mL/min after replacement.	Clogging of pipes in the old equipment.
KFR13	–	Clogging of pipes in previous equipment.
KFR7A	The previously observed pressure decrease with the old equipment was normalised following replacement.	Leakage and short circuiting between KFR7A:1 and KFR7A:2 .

Tabell 2-2. Borehole sections and identified deformation zones, modified from /8/.

Borehole idcode	Section	Section limits (m.b.l.)	Released packers	Penetrated deformation zone	Zone model geometrical intersection (m.b.l.)
KFR01	P1	44.5–62.3		Singö zone	0–62.3 (entire borehole)
	P2	11.0–43.5			0–62.3 (entire borehole)
KFR02	P1	137.0–170.3			
	P2	119.0–136.0		Zone H2	108.58–129.73
	P3	81.0–118.0		Zone H2	108.58–129.73
	P4	43.0–80.0			
	Blind	2.0–42.0		Zone 9A	32.89–36.88
KFR03	P1	81.0–101.6		Zone H2	79.87–101.02
	P2	57.0–80.0		(Zone H2)	
	P3	45.0–56.0		Zone 9B	51.51–54.76
	P4	5.0–44.0			
KFR04	P1	84.0–100.5		Zone H2	86.65–eoh, see comment
	P2	44.0–83.0			
	P3	28.0–43.0			
	P4	5.0–27.0		Zone 9B	21.08–23.94
KFR05	P1	97.0–131.4		Zone 9B	116.56–eoh
	P2	80.0–96.0		Zone H2	76.86–97.15
	P3	57.0–79.0		(Zone H2)	
	P4	12.0–56.0			
	Blind	4.0–11.0			
KFR7A	P1	48.0–74.7		Zone H2	24.05–eoh
				Zone 8	68.46–eoh
				Zone 0805b	50.32–61.2
	P2	20.0–47.0		Zone H2	
	P3	2.0–19.0			
KFR7B	P1	8.6*–21.1		Zone H2	6.92–eoh
	P2	4.0–7.6*		Zone H2	
KFR7C	–	0–34.4**	Yes**	Zone H2	14.12–eoh
KFR08***	P1	63.0–104.4		Zone 8	52.10–73.36
				0999	67.12–90.06
	P2	36.0–62.0		(Zone 8)	
				0805b	39.05–49.31
	P3	6.0–35.0			
KFR09	–	0–80.24	Yes**	Zone 3	41.42–eoh
KFR10	–	0–127.28	Yes**	Zone 3	71.48–eoh
				H2	70.56–94.03
KFR11****	–	0–98.07	Yes**	Zone 8	53.98–78.35
				0805b	29.03–40.56
KFR12	–	0–50.26	Yes**	Zone H2	15.37–36.52
KFR13	P1	54.0–76.6		Zone H2	49.83–70.99
	P2	34.0–53.0		(Zone H2)	
	P3	4.0–33.0			
KFR19	P1	95.0–110.17			
	P2	77.0–94.0			
	P3	66.0–76.0			
	P4	51.0–65.0			
	Blind	3.0–50.0			
KFR20	–	0–109.7			
KFR55	P1	49.0–61.89		(Zone 9b)	
	P2	40.0–48.0		Zone 9b	47.4–48.58
	P3	22.0–39.0			
	P4	8.0–21.0			
	Blind	6.0–7.0			
KFR56	P1	9.0–81.73		0805b	59.47–74.87

*These values are corrected by –0.6 m compared to initial information. During repair work of the downhole equipment in 1998, it was observed that the early information on packer locations was erroneous.

** Packers released between 1999 and 2000 (KFR09 and KFR10) and 1987and 1995 (KFR7C and KFR12). No documentation exists. Early samples originate from delimited sections.

*** No samples before 1989.

**** No samples after 1987.

2.3 Hydrogeochemical investigations

Sampling of groundwater in SFR boreholes for chemical analyses has been performed almost regularly from the construction phase in the middle of the eighties to the present day. The sampling activities/investigations are summarised in Table 2-3.

The first hydrogeochemical investigation (Investigation I) was performed by IMAB during the construction phase from 1984 to Oct. 1986 /3/ and /4/. The analytical programme was limited and included mainly major constituents and nutrient salts. Several shortcomings in the investigations resulted in unreliable data.

The following and more successful investigation (Investigation II) /4/, also carried out during the construction phase, was performed by SKB. The mobile laboratory and the hose unit with the Chemmac measuring system was used for analyses and on line measurements of pH, Eh, dissolved oxygen, electrical conductivity and water temperature. The on-line measurements were performed in three selected boreholes/borehole sections. Furthermore, the analytical programme was more extensive and included also isotopes for the same selected boreholes.

The control monitoring programme that was established for the operational phase in SFR has been running since 1989. The groundwater composition is checked regularly in four observation points/borehole sections in four different boreholes. Initially, this was done twice per year, but since 1996 the programme has been changed to once per year with more extensive sampling in all water yielding sections each fifth year, and also a more extensive analytical programme. Such extensive investigations have been performed four times but the complete dataset from the first occasion in 1992 unfortunately are not stored in Sicada. During year 2000 the mobile laboratory was used.

Table 2-3. Hydrogeochemical investigations in SFR-boreholes 1984 to present day.

Investigation	Time period	No. of samples	Comments
Investigation I	1984–Oct.1986	78	Questionable analytical results.
Investigation II	Nov. 1986–1987	56	Sampling/analyses performed by SKB from this period to present.
Control programme I	1989–1995	56	Sampling twice per year, 4 boreholes/borehole sections.
Control programme II	1996–forward	58	Sampling once per year, 4 borehole/borehole sections.
Extensive sampling	Years 1992, 1995, 2000 and 2006	118	Sampling in all water yielding borehole sections. Data from 1992 are partly lost.

3 Hydrogeochemical data

3.1 Available data

A total of 369 samples from 49 borehole sections in 19 SFR boreholes are recorded in the SKB database Sicada from 1984 to October 2007. The number of samples from each borehole section is listed in Table 3-1. From the total of 369, 278 records are complete regarding major constituents, deuterium and oxygen-18. These samples originate from two investigations during the construction

Table 3-1. Available data; sampled boreholes/borehole sections, number of samples, redox measurements, gas analyses and microbe determinations.

Idcode	Section (m)	Section no.	No of samples, < 1989	No of samples, ≥ 1989	Eh (years)	Gas (years)	Microbes (years)
KFR01	11.0–43.5	P2	2	4			
KFR01	44.5–62.3	P1	30	30	1987, 2000	2000	2000
KFR02	2.0–20.0	P6	3	–			
KFR02	21.0–42.0	P5	–	–			
KFR02	43.0–80.0	P4	4	4			
KFR02	81.0–118.0	P3	8	4			
KFR02	119.0–136.0	P2	1	4			
KFR02	137.0–170.3	P1	2	4			
KFR03	5.0–44.0	P4	1	4			
KFR03	45.0–56.0	P3	1	4			
KFR03	57.0–80.0	P2	3	3			
KFR03	81.0–101.6	P1	3	3			
KFR04	5.0–27.0	P4	–	1			
KFR04	28.0–43.0	P3	3	4			
KFR04	44.0–83.0	P2	–	4			
KFR04	84.0–101.0	P1	–	4			
KFR05	57.0–79.0	P3	–	2			
KFR05	80.0–96.0	P2	–	3			
KFR08	6.0–35.0	P3	–	4			
KFR08	36.0–62.0	P2	–	4			
KFR08	63.0–104.0	P1	–	28			
KFR09	0.0–80.2	P3	–	1			
KFR09	43.0–62.0	P2	1	–			
KFR09	63.0–80.2	P1	3	12			
KFR10	0.0–107.3	–	22	21	1987, 2000	2000	2000
KFR11	7.0 –24.0	P4	2	–			
KFR11	25.0–39.0	P3	2	–			
KFR11	40.0–55.0	P2	2	–			
KFR11	56.0–98.1	P1	13	–			
KFR12	0.0–50.25	–	–	1			
KFR12	20.0–33.0	P2?	1	–			
KFR13	4.0–33.0	P3	–	2			
KFR13	34.0–53.0	P2	–	4			
KFR13	54.0–76.6	P1	–	4			
KFR19	51.0–65.0	P4	–	1			
KFR19	77.0–94.0	P2	–	4			
KFR19	95.0–110.0	P1	–	3			
KFR20	0.0–109.7	–	–	1			
KFR55	8.0–21.0	P4	–	4			
KFR55	22.0–39.0	P3	–	4			
KFR55	40.0–48.0	P2	–	4			
KFR56	9.0–81.7	P1	–	4			
KFR7A	2.0–19.0	P3	–	4			
KFR7A	20.0–47.0	P2	–	3			
KFR7A	48.0–74.7	P1	19	30	1987, 2000	2000	2000
KFR7B	4.0–7.0	P2	–	4			
KFR7B	8.0–21.0	P1	2	4			
KFR7C	0.0–34.0	–	2	2			
KFR83	0.0–20.0		4	–			

phase of the SFR facility (77 +56 activities/samples) and from a control monitoring programme as a check of repository performance that has been running since 1989 (236 activities/samples). Sample series, together with on-line measurements of pH, Eh and electrical conductivity, are available from three borehole sections (KFR01:1, KFR10 and KFR7A:1) and from two different sampling campaigns in each borehole (1986–87 and 2000 respectively). Gas and microbe data have been obtained from the same three boreholes during the sampling campaign in 2000.

3.1.1 Uranium

Unexpectedly high uranium concentrations were observed in groundwater from some of the boreholes in the previous PLU investigations; this issue is still not resolved and further sampling and analysis are planned. Therefore, such anomalous uranium concentrations are of special interest also to the SFR facility and the planned investigations. Unfortunately, uranium has not been analysed frequently and the dataset contains only 7 values for U (µg/L) and 9 values for U-238 from 4 boreholes/borehole sections. The uranium concentrations and U-238 activities in the four boreholes are presented in Figure 3-1 and, as can be seen, the uranium concentrations are relatively high also in the SFR groundwaters.

3.1.2 Tritium

Reliable tritium values are rather scarce since data from 1993 to 1999 have been rejected due to sample contamination. Furthermore, the detection limit for early tritium data prior to 1999 was high and therefore less useful for comparison with later more precise values. From 1999 and onwards a laboratory with low enough detection limits has been used so that the same sample treatment and analysis relate to both SFR samples and, for example, the PLU samples. The sampling procedures and the analytical protocol should be equally reliable. Nevertheless, tritium values are often somewhat higher than expected and the reason for this is not fully understood and therefore the data should be used with great care. In the SFR facility contamination from the stored waste may be a possible explanation.

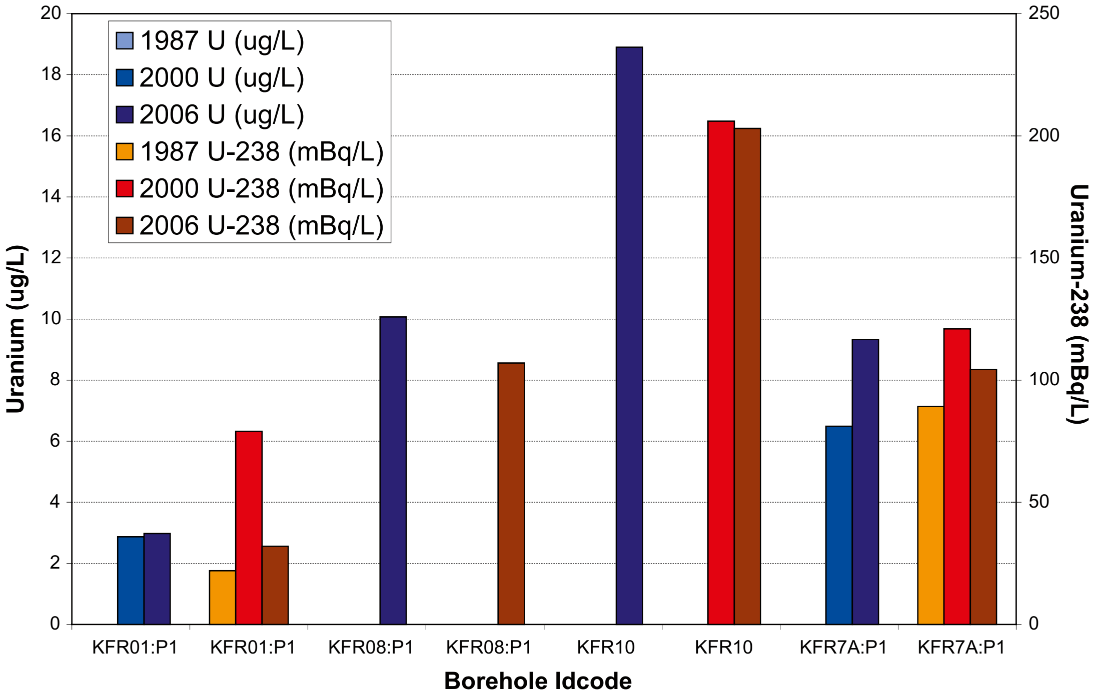

Figure 3-1. Available uranium data (concentrations and U-238 activities) in boreholes KFR01, KFR08, KFR10 and KFR7A. The samples were collected in 1987, 2000 and 2006.

3.2 Quality of hydrogeochemical analyses

3.2.1 General

The groundwater analyses treated in the present report have been carried out during more than twenty years and the analytical methods as well as the performing laboratories have changed several times during this time period.

The methods and quality of the groundwater analyses performed during the first and the second hydrogeochemical investigations in SFR (November 1984 to October 1986 and November 1986 to March 1987, respectively) are thoroughly discussed in /4/. The first investigation is also documented in /3/ but without any further comments on the quality of the analyses. It is clear from the scattered concentration values and the often unacceptably large charge balance errors that analytical data from the first investigation are less reliable, and this is also stated in /4/. Consequently, these samples have been classified as unsuitable for modelling in the data compilation presented in the SFR Hydrogeochemistry Table version 0.1. The second investigation was conducted using the SKB mobile laboratory and several samples were duplicated by a second laboratory as a check. The analytical performance improved considerably and the resulting hydrogeochemical data are considered to best represent the initial undisturbed conditions, i.e. unaffected or less influenced by the existence of the tunnel system than subsequent data. If not judged unsuitable for other reasons, these samples in the SFR Hydrogeochemistry Table version 0.1 have been classified as suitable for modelling.

Within the routine SFR groundwater monitoring programme focused on repository performance, the sampling and analyses that have been on-going since 1989 have been documented in yearly reports to the County Administrative Board and to SKI and in a few other comprehensive reports /5, 6/. In these reports the laboratories and analytical methods are thoroughly described but there is little focus on data quality. Generally, however, the methods used and the laboratories involved have been the same as in other contemporaneous hydrochemical investigations by SKB and the same checking procedures have been applied.

3.2.2 Measurement uncertainties, reporting limits and detection limits

A list of analytical methods, reporting limits and general measurement uncertainties as reported from the various contracted laboratories in 2008 is given in Table 3-2. The task to address the different analytical methods used and evaluate corresponding measurement uncertainties back to 1984 was considered to be both time consuming and not worthwhile. The uncertainties presently reported are supposed to include the time period from 1986, but nevertheless they can be presented independent of analytical methods and when the data were obtained, and therefore the values are included as error bars in the diagrams displayed in Figures 3-1 to 3-5. Although some detection limits probably have been improved upon since the early eighties, the assumptions regarding the measurement of uncertainties seem somewhat justified since: 1) reported uncertainties by the analytical laboratories have increased rather then decreased with time due to a more critical approach and change of estimation method according to more recently established and internationally accepted methods, and 2) from the second investigation (1986–1987) the different constituents show standard variations /4/ within the uncertainties given in Table 3-2.

Generally, all concentration values are reported down to the reporting limit (10×std). However, some late (after 2002) anion analyses performed by SKB were reported down to the detection limit (3×std) in order to facilitate further interpretation.

Table 3-2. Methods, reporting limits and measurement uncertainties (2008).

Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Meas. uncert.[3]	Comment
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]	After 2002
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]	After 2002
Na	ICP AES	0.1	mg/L	13%	Before 1989, AAS
K	ICP AES	0.4	mg/L	12%	Before 1989, AAS
Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Meas. uncert.[3]	Comment
Ca	ICP AES	0.1	mg/L	12%	Before 1989, AAS or titr
Mg	ICP AES	0.09	mg/L	12%	Before 1989, AAS or titr.
S(tot)	ICP AES	0.16	mg/L	12%	Start 1989
Si(tot)	ICP AES	0.03	mg/L	14%	Start 1989, before spectr.
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]	Start 1989
Mn	ICP AES	0.003	mg/L	12.1%[5]	Before 1989, spectrophotometric
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%	
NO_2 as N	Spectrophoto-metry	0.1	µg/L	2%	
NO_3 as N	Spectrophoto-metry	0.2	µg/L	5%	
NO_2+NO_3 as N	Spectrophoto-metry	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)	
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)	
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]	
Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Meas. uncert.[3]	Comment

Component	Method[1]	Reporting limits (RL), detection limits (DL) or range[2]	Unit	Meas. uncert. [3]	Comment
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	Before 1986, DL=3 TU, 1989 to 2000 DL= 8.4 TU
δ^{37}Cl	A (MS)	0.2	‰ SMOC[9]	0.2[16]	
δ^{13}C	A (MS)	–	‰ PDB[10]	0.3[16]	
^{14}C pmc	A (MS)	–	PMC[11]	0.4[16]	
δ^{34} S	MS	0.2	‰ CDT[12]	0.4 (one standard dev.)	
^{87}Sr/^{86}Sr	TIMS	–	No unit (ratio)[13]	0.00002	
^{10}B/^{11}B	ICP SFMS	–	No unit (ratio) [13]	–	
^{234}U, ^{235}U, ^{238}U, ^{232}Th, ^{30Th}	Alfa spectr.	0.0001	Bq/L[14]	≤ 5% (Counting statistics uncertainty)	
^{222}Rn, ^{226}Ra	LSS	0.015	Bq/L	≤ 5% (Count. Stat. uncert.)	

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[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 conductivity 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] Per mille deviation[15] from VSMOW (Standard Mean Oceanic Water).

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

[9] Per mille deviation[15] from SMOC (Standard Mean Oceanic Chloride).

[10] Per mille deviation[15] from PDB (the standard PeeDee Belemnite).

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

[12] Per mille deviation[15] from CDT (the standard Canyon Diablo Troilite).

[13] Isotope ratio without unit.

[14] 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.

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

[16] SKB estimation from duplicate analyses by the contracted laboratory.

3.2.3 Consistency checks and sources of analytical errors

In order to establish a consistent set of major constituent concentrations (mainly Na, Ca, Cl , SO_4 and possibly Mg and HCO_3) for each sample, the first step is to compare chloride concentrations and electrical conductivity (EC) values in x-y scatter diagrams. Figure 3-2 includes chloride concentrations and EC values (field-EC or lab-EC) and shows that the main part of the 143 data points (i.e. no. of samples having both chloride and EC values) follow the trend line indicating that the EC and chloride data sets are quite consistent. The most diverging points belong to samples from the first investigation, November 1984–October 1986. The relative charge balance gives an indication of the quality and uncertainty of the analyses of the major ions and, together with the chloride to EC correlation, they are used to verify that the concentrations of the most dominating ions are consistent. The errors, as calculated for the 290 samples with complete enough sets of major ions, exceed the acceptable limit ±5% in 39 cases, with all of them except one from the first investigation period from November 1984–October 1986.

The early groundwater data sets from the SFR boreholes do not offer too many possibilities to compare results from different methods and/or laboratories. Some of the samples from Investigation II were analysed by two laboratories and the evaluated best values were reported in the database at that time (Geotab).

Sulphate

From 2000 both sulphate and elemental sulphur were determined in each sample by Ion Chromatography (IC) and ICP-AES, respectively. The agreement between the two methods is reasonably good as shown in Figure 3-3. The ICP results generally show somewhat higher values which may be due to systematic analytical errors or effects from the presence of sulphide. This effect is not proportional to the sulphide-sulphur concentration as sulphide-sulphur enters the plasma as hydrogen sulphide gas.

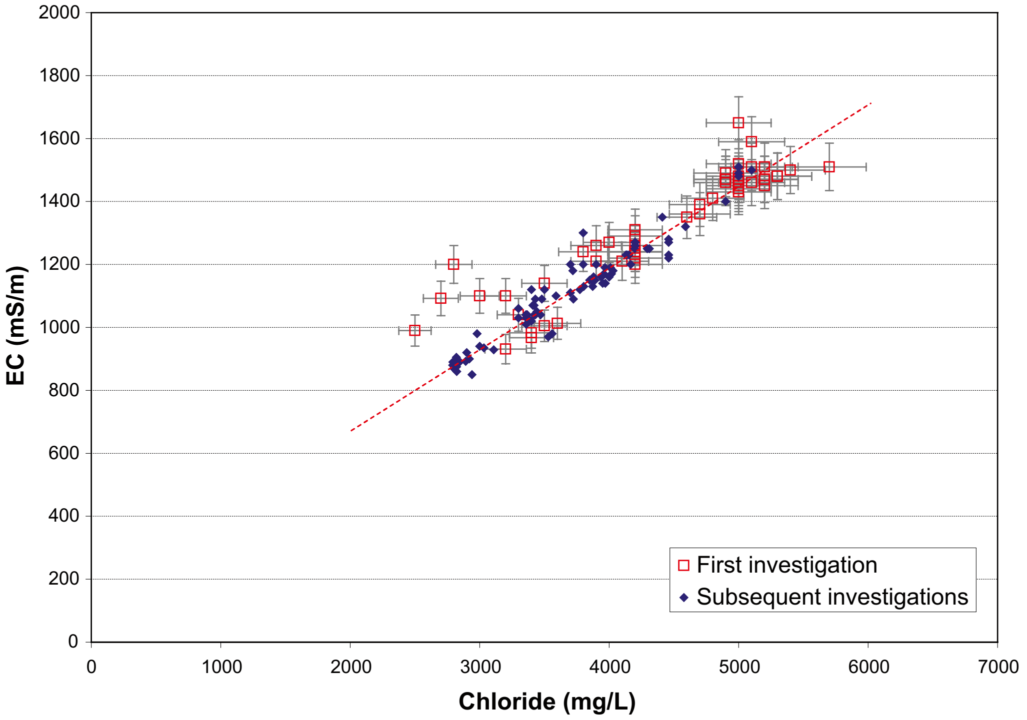


Figure 3-2. Chloride concentrations plotted versus EC values (143 samples)..

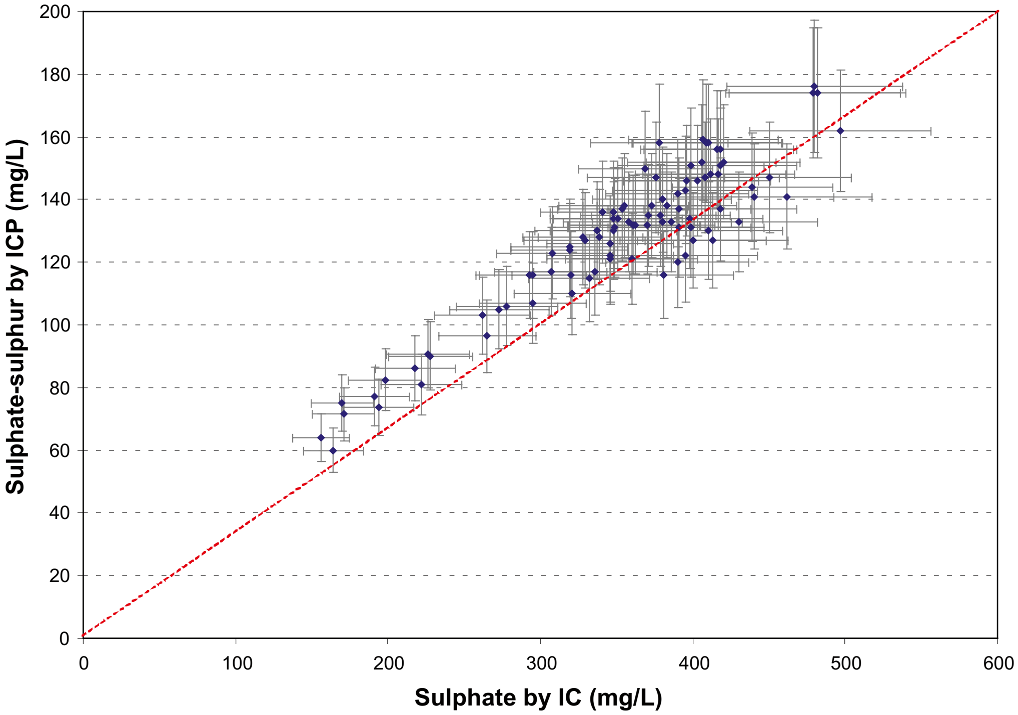


Figure 3-3. Comparison of sulphur by ICP-AES and sulphate by IC (91 samples). Without significant contribution of other sulphur species, 3×SO_4-S by ICP should correspond to SO_4 by IC.

Bromide

Bromide was not included in the first analytical programme from November 1984–October 1986 but was analysed in the next investigation which commenced in November 1986. Bromide concentrations are plotted versus the corresponding chloride concentrations in Figure 3-4 as a rough consistency check. The data points form an unusually scattered trend and it is difficult to detect any of the two often encountered trend lines in groundwater, i.e. the trend corresponding to a marine origin (Br/Cl slope close to 0.0035) and the trend more typical of water/rock interaction (Br/Cl slope approx. 0.01). The broad trend line may be due to the fact that all the sampled groundwaters are of mainly marine origin but more or less diluted by glacial melt-water. Furthermore, one bromide concentration deviates considerably and the value is most probably erroneous. The bromide analyses were impaired by larger uncertainty than most other major constituents and the dataset does not offer any possibility to compare results from two different methods.

Iron

A limited number of samples (41), all from 2000–2006, include values for both total/ferrous iron by spectrophotometry and elemental iron by ICP-AES. The agreement between the spectrophotometric and the ICP results is very good, see Figure 3-5. This is an indication that the presence of iron species in a colloidal phase is insignificant. The spectrophotometric method does not include, or only partly includes, eventual bounded iron that passes a 0.40 mm filter, but the ICP method makes no distinction between different iron containing species.

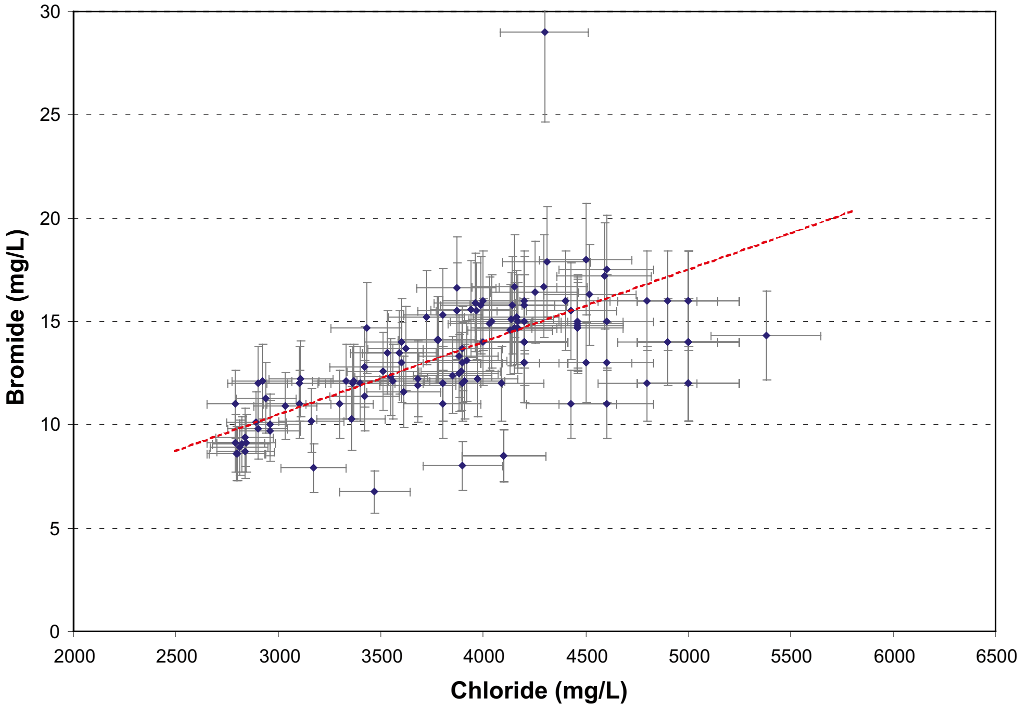


Figure 3-4. *Plot of bromide concentrations versus chloride concentrations (128 samples). The error bars correspond to ±15% and ±5% respectively. The red line has a slope of 0.0035=Br/Cl and ratios close to this value are typical for groundwaters of marine origin.*

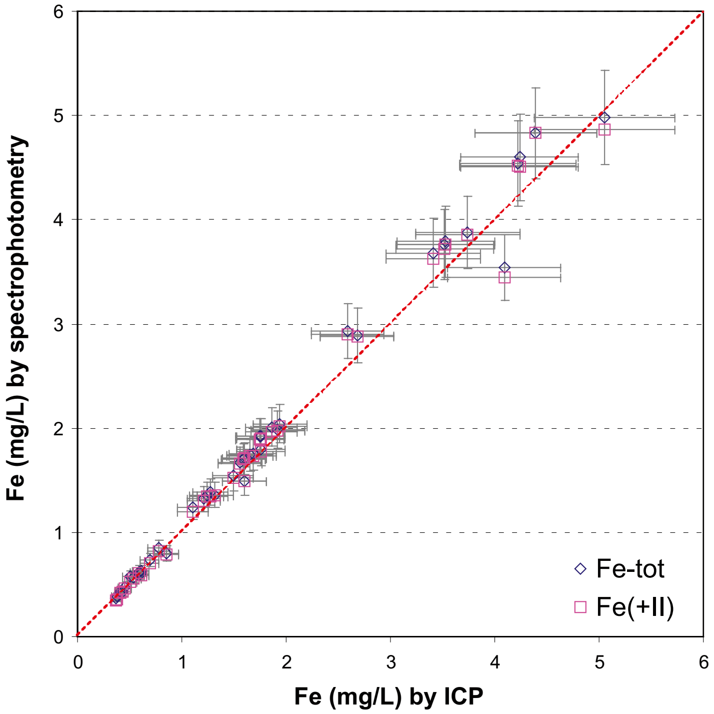


Figure 3-5. *Comparison of iron concentrations. Total and ferrous iron by a spectrometric method is plotted versus iron determined by ICP-AES technique (41 samples).*

3.3 Special measurements and experiments

3.3.1 Redox measurements

Redox measurements were conducted in1987 and repeated in the same three borehole sections in 2000:

- KFR01 section P1 (44.5–62.3 m).
- KFR7A section P1 (48.0–74.7 m).
- KFR10 section P1 (87.0–107.28 m) during 1987 and the entire borehole in 2000.

The measurement sequences for 1987 and 2000 are diagrammatically presented in Appendix 1. The mobile chemistry unit with the surface Chemmac measurement system was used for the measurements on both occasions. Modifications and improvements of the Chemmac system were performed later on prior to the PLU investigations. The outlet from the borehole section in the tunnel is connected directly to the Chemmac measurement cell and pumping is not required as the water is discharged by natural over-pressure. Generally, experience from similar redox measurements in boreholes from the Äspö HRL shows that the electrodes give stable and reliable readings faster than during corresponding measurements when groundwater is pumped to the ground surface. A possible reason for this disparity is that, in the latter case, no air-contaminated equipment is introduced into the borehole section. However, oxygen diffusion due to long tubing or poor choice of tubing material between the borehole and the measurement cell, placed in the tunnel close to the borehole orifice, may influence also tunnel borehole measurements. Detailed documentation regarding the experiment set-up is not available for the old SFR data, and therefore anomalously high redox potential values due to oxygen diffusion can not be excluded.

From the first occasion in 1987 only a few selected potentially suitable data are stored in Sicada, but not the full measurement sequences. Generally, the measurement results from both occasions are somewhat uncertain as they do not meet the quality criteria given by Gimeno et al. /10/. However, they may still provide some information on the groundwater system and some interpreted Eh values to be used with care are given in Table 3-3.

The first measurement in borehole KFR01 in 1987 resulted in reasonably stable negative potentials being registered by two electrodes (–133 and –139 mV). At the second measurement occasion in 2000, however, the three connected electrodes stabilised at a positive value between 80 and 120 mV for a 12 day period before starting to decrease to –100 mV after a further 20 days. This behaviour may be representative of the groundwater situation at the time rather than erroneous measurements.

The first measurement in borehole KFR7A in 1987 is more uncertain. One electrode showed the expected measurement trend and stabilised at a potential of –177 mV, but the second electrode showed an increase from –236 to –143 mV during the first four days of the measurement sequence. At the last occasion in 2000 all three electrodes stabilised at a positive Eh between 10 and 50 mV. Also in this case, a positive Eh may be representative of the true groundwater situation at the time, and if the measurements had continued it is also possible that a similar decrease in Eh would have been registered as in borehole KFR01.

The more or less stable period recorded from early measurements in borehole KFR10 lasted almost 50 days. In spite of this long measurement period, the different electrodes stabilised at different positive or close to zero potential values (–10 to 105 mV). However, it is common to record diverging electrode readings when redox potentials are close to zero, and also the late measurements showed positive redox potentials which were stable and reproducible (60 to 90 mV).

Table 3-3. Summary of Eh values (Standard Hydrogen Electrode) given as a comment in the data compilation version 0.1 (to be used with care).

Borehole	Section	Interpreted Eh 1987 (mV)	Interpreted Eh 2000 (mV)
KFR01	P1, 44.5–62.3 m	–140	Changing due to discharge
KFR7A	P1, 48.0–74.7 m	–180	+20
KFR10	P1, 87.0–107.28 m	Approx. 0	+80 (entire borehole)

3.3.2 Microbial investigations

Although data from microbial investigations in 2000 are too few for further evaluation, they may be useful for comparison together with new microbe data from ongoing investigations. The results from the 2000 investigations are documented in /5/.

3.3.3 Gas sampling and analyses

In common with the microbes, data from gas sampling and analyses in 2000 are too few for further evaluation, although they may be useful for comparison together with new gas data from ongoing investigations. The results from the 2000 investigations are documented in /5/.

3.4 Representativity classification

All SFR samples are collected from tunnel boreholes where the water flow is directed towards the tunnel and therefore there is little risk of contamination from drilling, drilling water or other borehole activities. However, trends in groundwater composition have been observed when sample series were collected during continuous discharge from a borehole. Discharge from boreholes may cause mixing of groundwaters with different origins and compositions, and differences in extracted volumes may lead to variation in concentrations that could be misinterpreted.

In addition, the presence of the tunnel system has an impact on the hydrogeological conditions in terms of changed flow paths and groundwater drawdown effects. These effects are observed from long term hydrochemical trends as very slow but systematic changes in the groundwater composition, i.e. dilution with modern marine water from the Baltic Sea. This slow dilution is mainly observed in boreholes intersecting major vertical deformation zones.

The dataset including samples collected between 1984 and 2007 has been evaluated systematically with respect to quality and an assignment was made with respect to their value for further hydrogeochemical interpretation work using a similar approach as /7/. However, the conditions that need to be considered in this case are somewhat different from the PLU dataset and therefore the categorisation criteria will differ also. To denote the SFR groundwater samples, Latin numerals are used instead of Arabic numerals to differentiate between the five categories. Categories I–III primarily meet the requirements of hydrogeochemical (but also hydrogeological) modelling of initial, or at least nearly initial conditions. Category IV primarily meets hydrogeological requirements but also hydrogeochemical requirements concerning effects from the tunnel on groundwater chemical conditions and groundwater development during the operational phase. Category V data need to be used with great caution in the context of both hydrogeochemistry and hydrogeology.

The most important criteria used to categorise the groundwater samples are listed in Table 3-4 and more detailed descriptions of each sample category are given in the text below.

Category I Samples: Selected samples from Investigation II. Satisfactory sample series data (i.e. stable chemistry recorded over several days to weeks), complete major ions and environmental isotopes (^{2}H and ^{18}O), acceptable charge balance, a good coverage of trace constituents and measurement of redox potential.

Category II Samples: Samples from Investigation II. Satisfactory sample series data (i.e. stable chemistry recorded over several days to weeks), complete major ions and environmental isotopes (at least ^{2}H and ^{18}O), acceptable charge balance, a good coverage of trace constituents for some of the samples in the series.

Category III Samples: Samples from an inadequate or unstable sample series or a long term time series. Also, samples that lack a few major ion data but still allow a reasonable charge balance calculation.

Category IV Samples: All samples collected during the operational phase from 1989 and onwards and single samples (no sample series or time series) from Investigation II. Samples or sample series without environmental isotope data. *Category IV samples may be used to evaluate the development of the groundwater conditions that are due to the existence of the tunnel system.*

Category V Samples: All samples collected during Investigation I as well as samples with some important major ions missing and samples with an unacceptable charge balance.

Table 3-4. Categorisation criteria for groundwater data representing early sampled boreholes in the SFR-tunnel system.

Boreholes **Aspects/Conditions**	**Category**				
	I	**II**	**III**	**IV**	**V**
Initial/early sample from investigation I					x
Initial/early sample from investigation II	x	x	x	x	x
Sample from control programme during operation of SFR				x	x
Sample series adequate and stable	x	x	x	x	x
Sample series inadequate or unstable			x	x	x
Time series			x	x	x
Sample series and time series absent				x	x
Charge balance within ±5%	x	x	x	x	x
Charge balance not within ±5%					x
Major ions complete	x	x	x	x	x
Major ions incomplete (allow charge balance calculation)			x	x	x
Major ions incomplete (do not allow charge balance calculation)					x
Environmental isotopes available (at least ^2H and ^{18}O)	x	x	x	x	x
Environmental isotopes not available				x	x

Explanations:

Investigation I = Sampling period 1984–Oct.1986.

Investigation II = Sampling period Nov. 1986–1987.

Control programme = Sampling once or twice per year during the operational phase from 1989 and onwards.

Sample series = Several or frequent samples collected during a period of days or weeks. The water is constantly discharged from the borehole section until the sampling series is collected.

Time series = Regularly collected samples during several months or years. The valve to the borehole section is closed and discharge from the borehole section is interrupted in between the sampling occasions.

4 Hydrogeochemical data presentation

4.1 3D visualisation

Distributions of chloride and magnesium concentrations as well as oxygen-18 signatures in the SFR-repository bedrock volume are presented in 3D in Appendix 2. Both initial/early (1987) and operational (2006) conditions are displayed. The 3D presentations are based on the updated SFR repository design 2008, the preliminary DZ-model version 0.1 from 2008-12-20, and the SFR Hydrochemistry Table version 0.1.

The spatial distribution of chloride concentrations provides a basic understanding of the hydrogeochemical conditions at the SFR investigation site. The saline component may originate from relict (Littorina) and modern (Baltic) Sea water or possibly deeper saline groundwater /6/. In the SFR groundwater system, the contribution from modern brackish Baltic Sea water causes dilution of the groundwater.

High magnesium and sulphate concentrations, as well as a low bromide to chloride ratios, indicate a marine origin of the groundwater. Ion exchange processes in the bedrock fracture systems may weaken the marine water signature by causing a decrease in Mg and Na and an enrichment of Ca. In Forsmark, the previously observed /7/ clear difference in magnesium concentration between waters of Littorina type and non-marine groundwaters indicates that the effect of ion exchange is not significant enough to prohibit the use of magnesium concentrations to qualitatively interpret marine contributions. A cut-off value of greater than 25 mg/L Mg has been used in the PLU investigations to indicate a marine component.

A high or enriched $\delta^{18}O$ value generally indicates a marine origin and lower or depleted $\delta^{18}O$ values for the deeper, more saline groundwaters, indicates a distinct cold climate recharge (glacial) component (i.e. < –13‰ VSMOW). However, water-rock interaction also increases the $\delta^{18}O$ values in the deeper groundwaters, which complicates interpretation. The modelled $\delta^{18}O$ value for Littorina Sea water is –4.7‰ VSMOW while the value for fresh glacial meltwater is –25‰ VSMOW. Groundwaters from intermediate depths in Forsmark with chloride concentrations of around 4,000–5,500 mg/L and $\delta^{18}O$ values between –9 and –12‰ VSMOW have been interpreted as Littorina Sea/glacial water mixtures /7/.

Two sets of figures showing initial/early and late conditions (2006) are given in Appendix 2 and organised to facilitate comparison and identification of changes in groundwater composition with time. Due to the low quality of the analyses from the first sampling campaign (Investigation I), most of the presented initial data originate from the second sampling campaign Nov. 1986–1987 (Investigation II). The visualised data from the operational phase originate from the extensive investigations carried out in 2006. Samples used for 3D representation are identified in the Hydrogeochemistry table version 0.1 in the column '3D visualisation'. The following selection criteria were used for visualising initial/early data:

1. Chloride and magnesium data are initially selected from samples categorised as the most representative from the Investigation II data series.
2. For the chloride distribution, complementary information from Investigation I data are used for borehole sections which lack data from Investigation II, i.e. if both chloride and EC values are available and consistent, and if the charge balance agrees within ±5%.
3. The oxygen-18 distribution is based on the 1995 dataset since earlier oxygen-18 data are sporadic and scarce.

4.2 Long term trends

Chloride, magnesium and oxygen-18 data resulting from around twenty years of groundwater sampling in the SFR repository bedrock volume are presented as x/y scatter diagrams versus sampling date in Appendix 3. All data, including the low quality data prior to Nov. 1986 (Investigation I) are used in the plots. The concentration trends are plotted borehole by borehole. Boreholes with at least one borehole section that has been sampled on more than three occasions are presented. The diagrams display major changes in the groundwater composition with time and also differences between the different borehole sections.

Observations from the long term trends are summarised as follows:

- Clear but slow changes in the groundwater composition, implying decreases in chloride and magnesium concentrations and increases in $\delta^{18}O$ values, most probably due to introduction of present Baltic Sea water, are observed in boreholes KFR01 (both sections), KFR7A, KFR7B, KFR09 and KFR10.
- Less significant changes or stable compositions are observed in boreholes KFR02A, KFR03, KFR04 and KFR08.
- Borehole KFR11 shows a practically stable groundwater composition during the short sampling period from Jan.1986–March 1987.
- A possible effect from the intersection of deformation zone H2 on the groundwater composition (increase in Cl and Mg and decrease in $\delta^{18}O$ values) is observed in borehole KFR02 section P2 and possibly P3, borehole KFR03 section P1, and borehole KFR04 sections P1and P2.

4.3 Data presentation in x/y scatter plots

As described in section 4.1, the magnesium concentration may be used to qualitatively interpret the marine contribution to the groundwater composition and a low or depleted $\delta^{18}O$ origin (< –13‰ VSMOW) indicates a glacial meltwater origin. In Appendix 4, magnesium and $\delta^{18}O$ are plotted versus chloride concentration to illustrate the variation in groundwater composition and mixing of different groundwater types in the different sampling locations; samples of category I to IV are included. The magnesium and $\delta^{18}O$ data are plotted twice, one including deformation zone labels and the other borehole idcode labels.

All the groundwaters encountered in the SFR-boreholes contain a marine component (Littorina or present Baltic Sea) /7/. In Figures A5-1 and A5-2 the magnesium versus chloride plots display a clear mixing line between marine waters of Littorina origin and present marine water. The magnesium concentrations are somewhat lowered compared to pure mixing between interpreted Littorina water and today's Baltic Sea water, probably due to ion exchange. The data points in the two diagrams can be divided into three groups; 1) those composing the mixing line, 2) an intermediate group, and 3) those deviating from the mixing line. Furthermore, SFR-groundwaters may contain a glacial meltwater component. In Figures A5-3 and A5-4 the $\delta^{18}O$ versus chloride diagrams display a triangle formed by the Littorina-Baltic Sea mixing line, the Littorina-glacial meltwater mixing line, and mixing in between those lines. Also, here the data points can be divided into three groups; 1) those composing the mixing line between the Littorina and present marine water, 2) an intermediate group, and 3) those composing the Littorina–glacial meltwater mixing line.

The boreholes or borehole sections with groundwaters belonging to group 1, 2 or 3, in the case of magnesium as well as in the case of $\delta^{18}O$, all, coincide. In Table 4-1 the boreholes included in each group are given.

Differences in groundwater composition and in the oxygen-18 signature between sections of the same borehole when intersecting deformation zone H2 can be clearly observed in boreholes KFR02, KFR13, KFR03 and KFR04. In these four boreholes, the chloride and magnesium concentrations increase and $\delta^{18}O$ decreases when intersecting zone H2.

Table 4-1. Simple grouping of boreholes/borehole sections into groundwaters with a strong marine signature (Group 1), intermediate waters representing mixing from group 1 and 3 (Group 2), and groundwaters showing a significant glacial component (Group 3).

Group	Borehole	Section	Zones	Comment
1	KFR7A	P1	Zone H2, zone 8 and zone 0805b	
		P2	Zone H2	
		P3	No zone	
	KFR7B	P1	Zone H2	
		P2	Zone H2	
	KFR08	P1	Zone 8, 0999	
		P2	Zone 8, 0805b	
		P3	No zone	
	KFR09	–	Zone 3	
	KFR10	–	Zone H2 and zone 3	
	KFR11	P1	Zone 8	Section P3 belong to Group 2
		P2	Zone 8	
		P4	No zone	
	KFR19	P1–P4	No zone	
	KFR20	–	No zone	
	KFR56	P1	zone 0805b	
2	KFR01	P1	Singö zone	
		P2	Singö zone	
	KFR04	P1	Zone H2	
		P2	No zone	Section P3 belong to Group 3
	KFR05	P2	Zone H2	
		P3	Zone H2 partly	
	KFR7C	–	Zone H2	
	KFR11	P3	Zone 0805b	Section P1, P2 and P4 belong to Group 1
	KFR12	–	Zone H2	
	KFR55	P1	Zone 9B partly	
		P2	Zone 9B	
		P3	No zone	
3	KFR02	P1	No zone	
		P2	Zone H2	
		P3	Zone H2	
		P4	No zone	
	KFR03	P1	Zone H2	
		P2	(Zone H2)	
		P3	Zone 9B	
		P4	No zone	
	KFR04	P3	No zone	
	KFR13	P1	Zone H2	Group 2 in the δ^{18}O case
		P2	(Zone H2)	
		P3	No zone	
	KFR83	–	–	Uncertainty about data

4.4 Depth trends

Concentrations of Na, Ca, Mg, Cl, HCO_3 and SO_4 (categories I to IV) are presented as a function of elevation in Appendix 5. The same division into groups as in section 4.3 has been used in order to check if this simple division based only on magnesium and $\delta^{18}O$ correspond with the other components. Furthermore, the grouping will make it easier to observe depth trends and also to reveal erroneous analytical data. The components selected are those frequently analysed and the most likely ones to show depth trends. The sulphate diagram presents sulphate data obtained by ion chromatography and excludes sulphate-sulphur by ICP.

Some observations:

- Na, Ca, Cl and SO_4 concentrations from borehole KFR83, at 92.94 m below sea level, deviate from the rest of the group 3 data. In this case the group division is based only on magnesium concentration. These early magnesium concentrations may be erroneous (too low), however, the bicarbonate concentrations support the group 3 type water.
- The Mg concentration of the single sample from borehole KFR12 at 113.62 m below sea level is possibly too high since it deviates from the rest of the dataset, see also Appendix 4, Figure A4-1.
- Two single samples from sections P3 and P4 in borehole KFR11 show deviating bicarbonate and sulphate concentrations from their group. $\delta^{18}O$ data are not available and the grouping is based only on magnesium.
- Calcium and chloride concentrations show clear increasing trends with depth.
- Sodium, magnesium and sulphate concentrations are divided into two separate trends according to which group they belong to; increasing trends are not that clear.
- The bicarbonate concentration is expected to decrease with depth. This is possibly the case for group 1 data, but not for group 3 data which indicate an increase with depth.

5 Discussion and summary

5.1 Dataset

Sampling and analyses of groundwater from the SFR boreholes have been carried out during more than twenty years. During this time the sampling personnel, analytical programme, analytical methods as well as the performing laboratories, have changed several times and naturally the quality of the data varies. The total amount of data from this extensive time period are compiled in the SFR Hydrogeochemistry Table version 0.1 which is stored in SKBDoc for subsequent use in the modelling group. The samples/data records in the table are quality controlled into different categories resulting in a range of judged values for continued hydrogeochemical interpretation work. Some comments on the dataset are listed below:

- The total dataset from boreholes in the present SFR is patchy and irregular. Especially the early data from 1986–87 and 1992 may lack several useful components for modelling purposes. Early tritium data should not be used due to the high detection limit.
- Borehole sections intersecting major deformation zones are sampled more frequently than other boreholes and borehole sections representing single fractures or minor fracture zones.
- The quality of the analytical data from the first hydrogeochemical investigation in SFR is not acceptable for modelling purposes.
- Data from the second investigation, performed by SKB from Nov. 1986–1987, are generally suitable for modelling and should be used to represent initial conditions before the operational phase in the SFR facility started. The analytical methods were different from today but the quality of the analyses documented in detail at that time, have been found to be sufficiently acceptable in the present evaluation.
- Other possible reasons for inconsistent data besides analytical errors, for example, sample confusion, printing mistakes and errors arising from the transfer of data between databases, can not be excluded, but most of the questionable data should have been removed from the present evaluation.

5.2 Groundwater composition and water types

As already stated in /6/, the groundwaters encountered in the boreholes drilled from the SFR tunnel system generally have a mainly marine origin (Littorina or present Baltic Sea) with varying contributions from glacial meltwater. In the present evaluation some indications of influence between groundwater data and geological entities (i.e. deformation zones) are observed. The groundwaters are divided, based on only magnesium concentration and $\delta^{18}O$ ratio, into three groups: 1) groundwaters with a strong marine signature, 2) intermediate groundwater mixtures *(between group 1 and 3),* and 3) groundwaters with a significant glacial contribution. All groups are related to their proximity to the intersected deformation zones. The following observations are made:

- Generally, the most marine type of water is found within or close to vertical deformation zones (e.g. zone 3 and zone 8) or where these zones intersect the gently dipping zone H2.
- The most saline water is of the marine type and is encountered at depth in zone 8 and zone 3.
- The groundwater encountered in the Singö zone is an example of an intermediate mixture.
- The groundwaters with the most significant contribution of glacial meltwater are found at some distance from zone 8 and zone 3 and above zone H2.
- In a borehole section representing zone H2, the chloride and magnesium concentrations generally increase and the $\delta^{18}O$ ratio decreases compared to the rest of the delimited sections in the same borehole. This is due to a larger contribution of Littorina type water. Generally, the water belongs to the group constituting the Littorina–glacial meltwater mixing line.

5.3 Changes in water composition with time

The impact of changes in flow paths and groundwater drawdown effects from the tunnel system will affect the groundwater composition in the SFR boreholes with time. These effects are observed from long term trends such as very slow but systematic changes in the water composition, e.g. dilution with modern marine water from the Baltic Sea /6/. Some comments on the observations are presented below:

- The true initial groundwater composition in each borehole/borehole section is not really known. The earliest sampling activity resulted in less reliable data classified as unsuitable for modelling purposes and, furthermore, by then the presence of the tunnel system may have affected already the groundwater composition.
- The largest changes in the groundwater composition are observed in boreholes KFR01, KFR09, KFR7A and KFR7B and to some extent in borehole KFR10. The groundwaters generally belong to group 1 waters with a strong marine signature. Borehole KFR01, in group 2, is an exception. However, the fact that the entire borehole represents the Singö zone may explain that changes occur also in this borehole.
- In boreholes KFR02, KFR03 and KFR04 the changes in water composition are small or insignificant. The groundwaters in these boreholes, generally represent group 3 (significant glacial meltwater contribution) and the mixing line groundwaters between Littorina water and glacial meltwater.
- Borehole KFR08 is another borehole with small or insignificant changes of the groundwater composition. This groundwater is the one that most resembles present marine water from the start. The first samples were, however, collected as late as 1989 and changes may have occurred already by then.

6 References

/1/ **SKB, 2008a.** Geovetenskapligt undersökningsprogram för utbyggnad av SFR. SKB R-08-67, Svensk Kärnbränslehantering AB.

/2/ **SKB, 2008b.** Bedrock hydrogeochemistry, Forsmark Site Descriptive Model. SKB R-08-47, Svensk Kärnbränslehantering AB.

/3/ **Grundvattenkemi i SFR.** SKB SFR 86-05. Svensk Kärnbränslehantering AB.

/4/ **Laurent S, 1991.** Vattenanalyser i SFR 1984–1986. Kvalitetsgranskning av data. SKB AR 91-23. Svensk Kärnbränslehantering AB.

/5/ **Nilsson A-C, 2002.** Grundvattenkemi i SFR. Resultat av provtagnings- och analyskampanj under år 2000. SKB R-02-21, Svensk Kärnbränslehantering AB.

/6/ **Laaksoharju M, Gurban I, 2003.** Groundwater chemical changes at SFR in Forsmark. SKB R-03-03, Svensk Kärnbränslehantering AB.

/7/ **Smellie J, Tullborg E-L, Nilsson A-C, Sandström B, Waber N, Gimeno M, Gascoyne M, 2008.** Explorative analysis of major components and isotopes. SDM-Site Forsmark. SKB R-08-84. Svensk Kärnbränslehantering AB.

/8/ **Curtis P, Petersson J, Triumf C-A, 2009.** Site investigation SFR. Deformation zone modelling. Model version 0.1. SKB P-09-48. Svensk Kärnbränslehantering AB.

/9/ **Öman J, Follin S, 2009.** Site Investigation SFR. Hydrogeological modelling of SFR. Data review and parameterisation of model version 0.1, SKB P-09-49. Svensk Kärnbränslehantering AB.

/10/ **Auqúe L, Gimeno M J, Gómez J, Nilsson AC, 2008.** Potentiometrically measured Eh in groundwater from the Scandinavian Shield. Applied Geochemistry 23 (2008) 1820–1833.

Appendix 1

On-line redox measurements

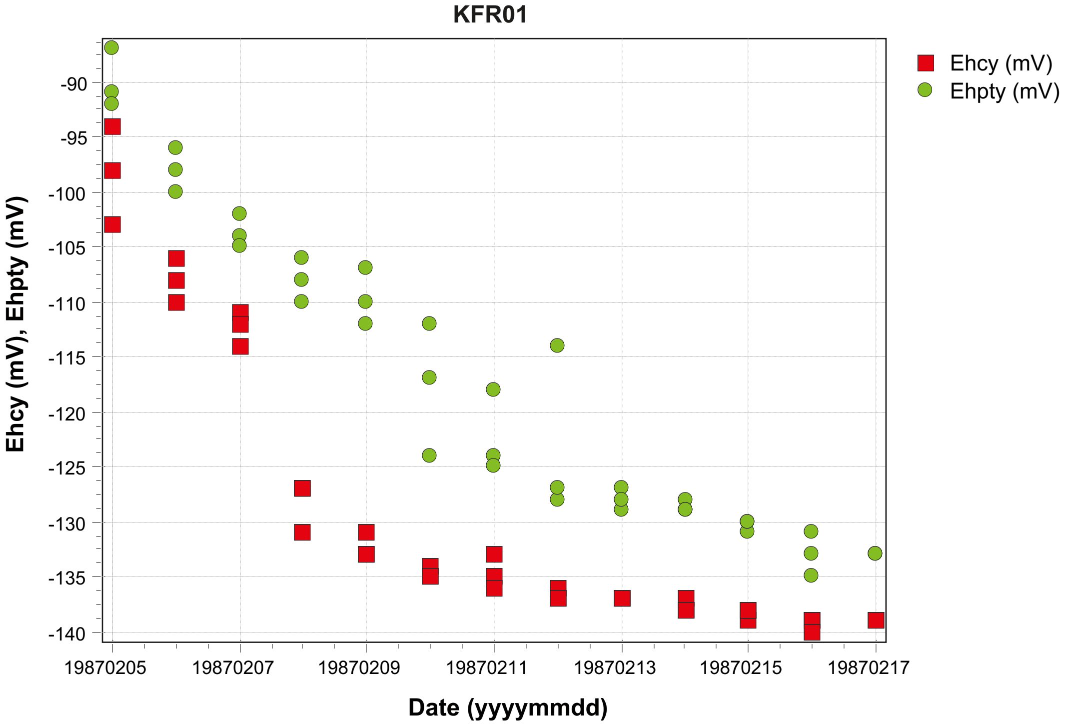


Figure A1-1. *Early redox measurements in borehole KFR01 section 44.5–62.3 m.b.l. during 1987. A glassy carbon electrode (Ehcy) and a platinum electrode (Ehpty) were used for the measurements.*

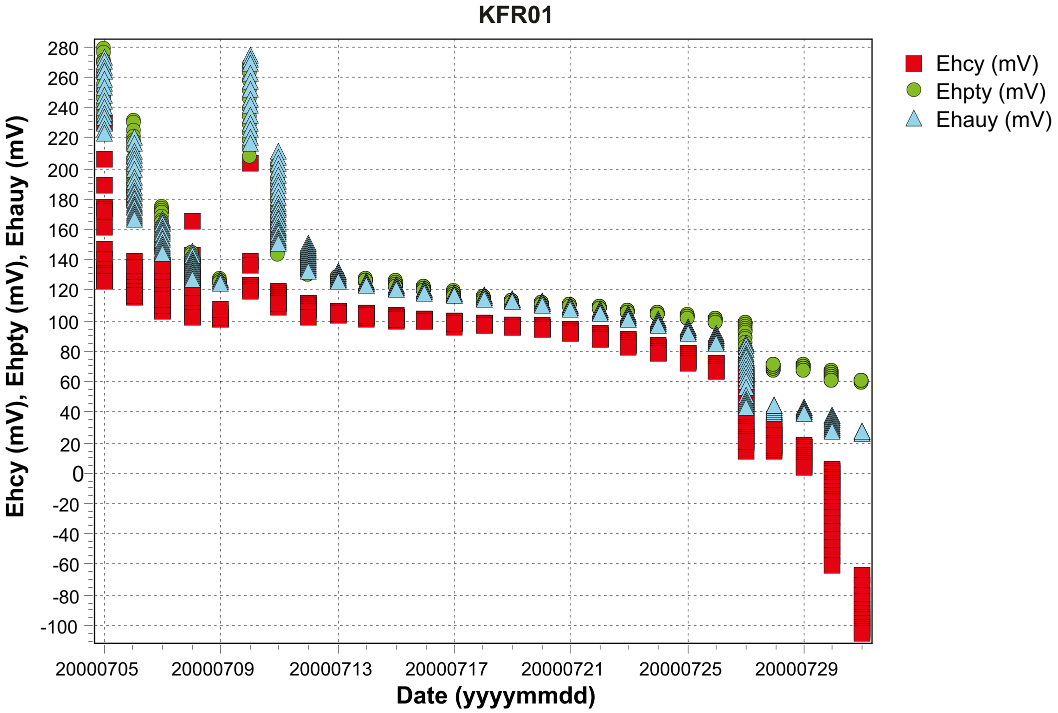


Figure A1-2. *Redox measurements in borehole KFR01 section 44.5–62.3 m.b.l. during 2000. A glassy carbon electrode (Ehcy), a platinum electrode (Ehpty) and a gold electrode (Ehauy) were used for the measurements.*

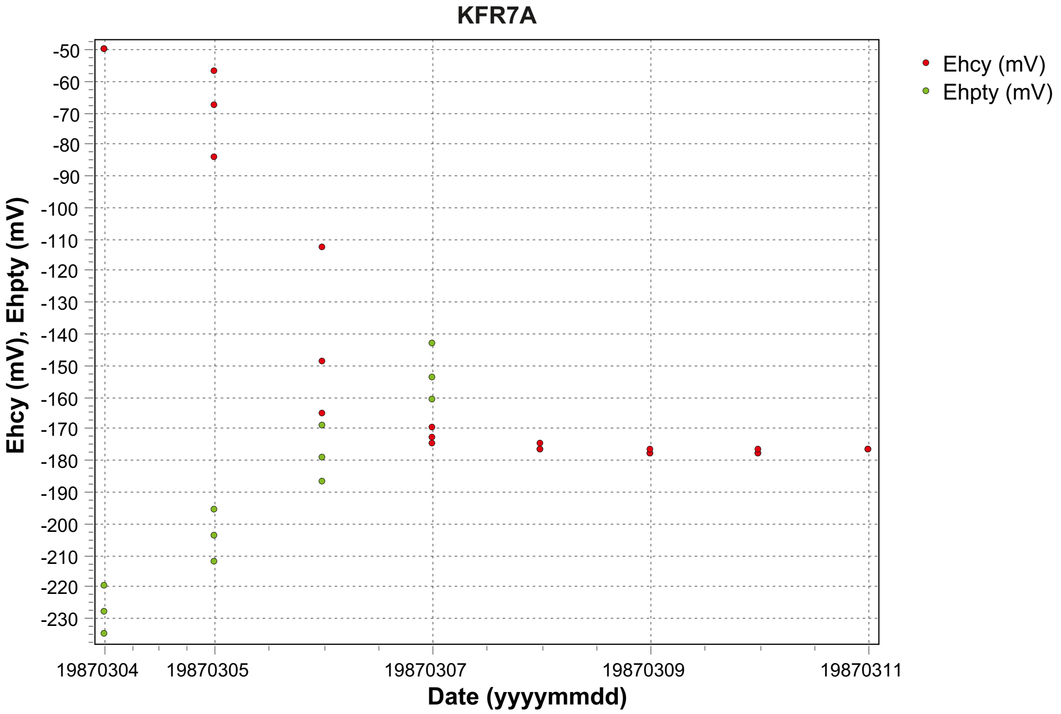


Figure A1-3. *Early redox measurements in borehole KFR7A section 48.0–74.7 m.b.l. during 1987. A glassy carbon electrode (Ehcy) and a platinum electrode (Ehpty) were used for the measurements.*

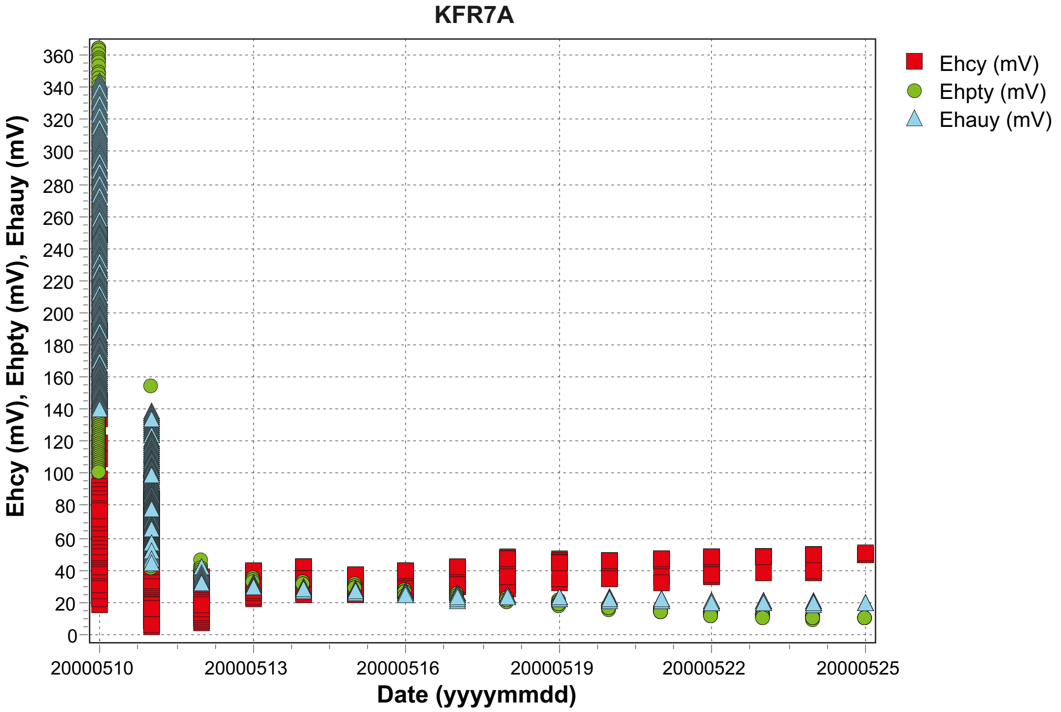


Figure A1-4. *Redox measurements in borehole KFR7A section 48.0–74.7 m.b.l. during 2000. A glassy carbon electrode (Ehcy), a platinum electrode (Ehpty) and a gold electrode (Ehauy) were used for the measurements.*

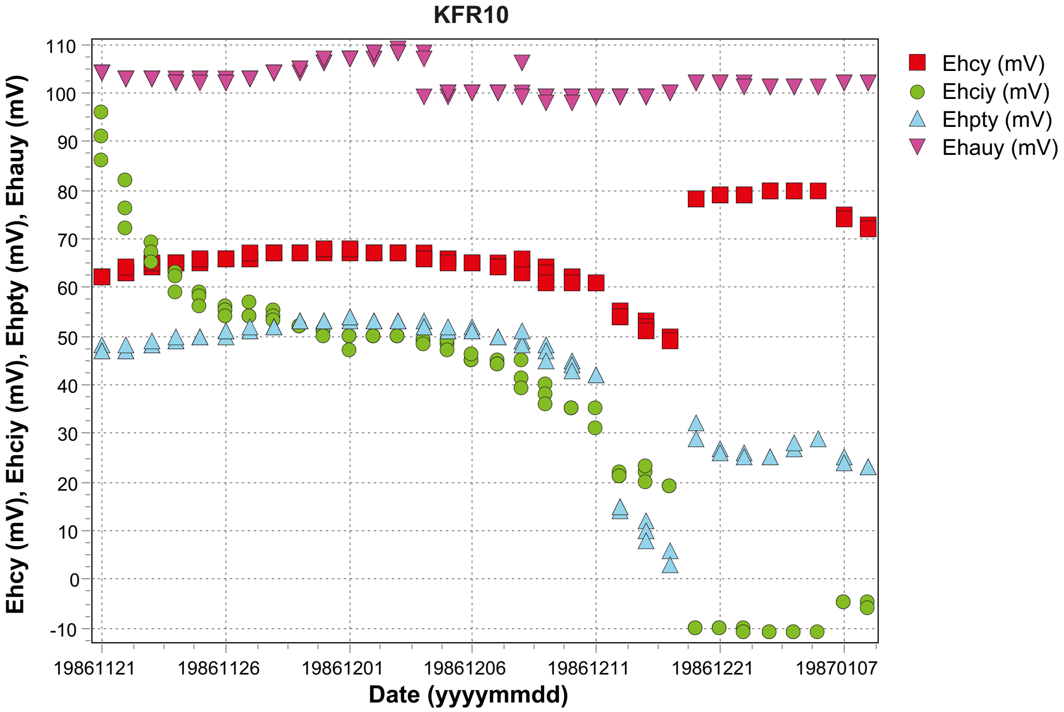


Figure A1-5. *Early redox measurements in borehole KFR10 section 87.0–107.28 m.b.l. during 1986. Two glassy carbon electrodes (Ehcy and Ehciy), a platinum electrode (Ehpty) and a gold electrode were used for the measurements.*

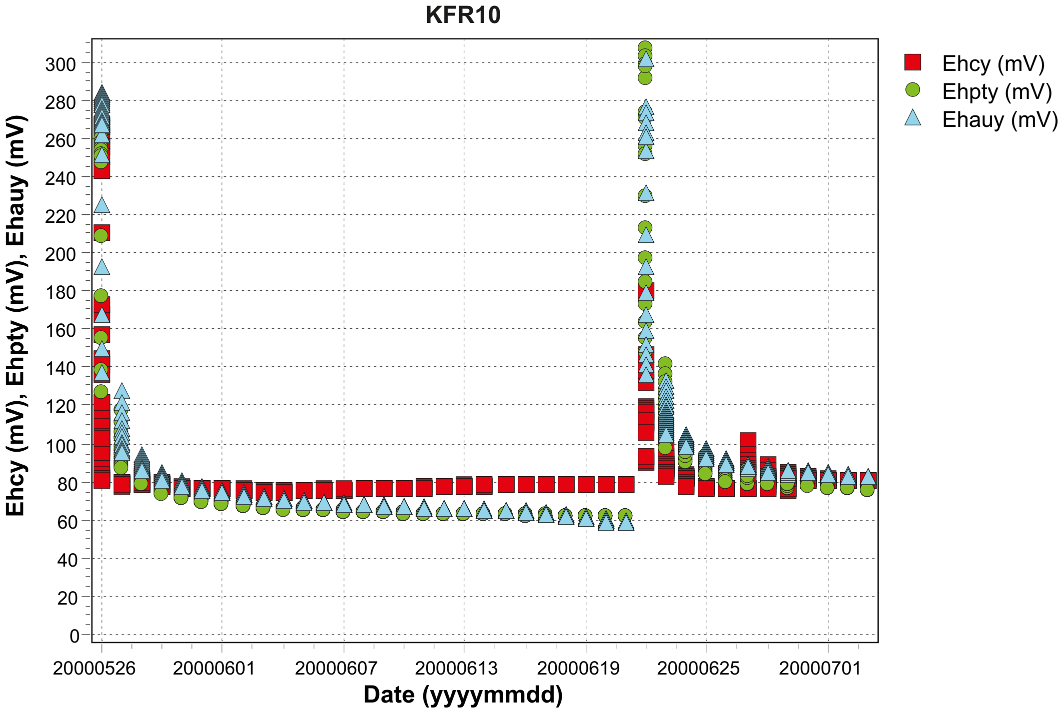


Figure A1-6. *Redox measurements in the entire borehole KFR10 during 2000. A glassy carbon electrode (Ehcy), a platinum electrode (Ehpty) and a gold electrode (Ehauy) were used for the measurements.*

Appendix 2

3D visualizations of Chloride and Magnesium concentrations as well as Oxygen 18 ratio in SFR-boreholes

The concentration intervals are indicated by colour and by diameter of rod as an elucidation in cases of similar colours.

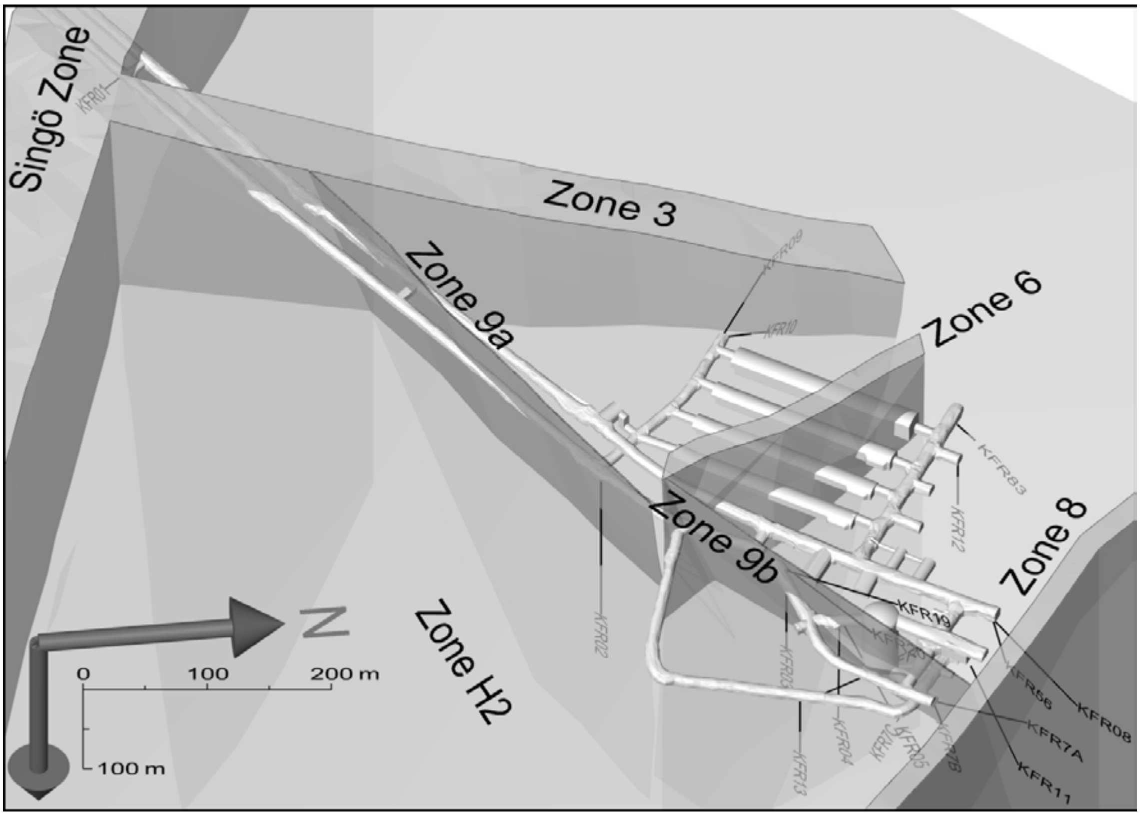


Figure A2-1. Overview in 3D of today's tunnel system in SFR with deformation zones and boreholes (no perspective distortion of size).

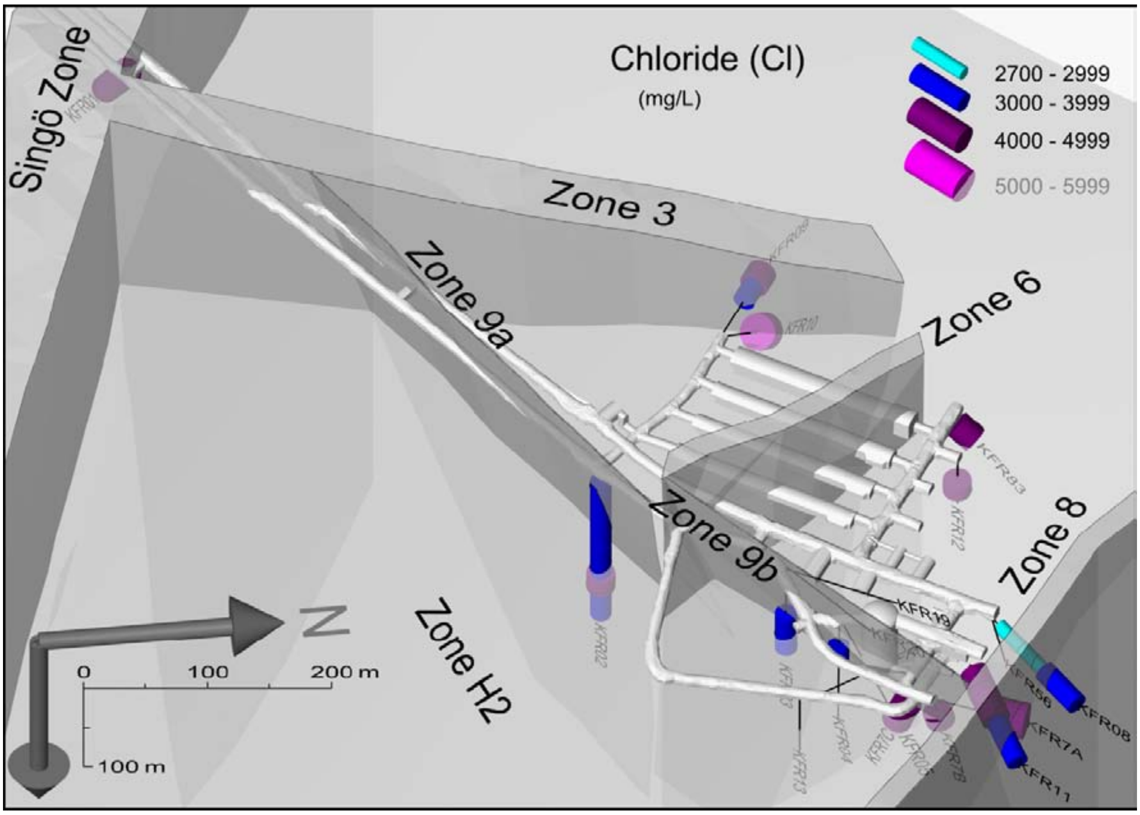


Figure A2-2. *SFR tunnel system, deformation zones and initial chloride concentration (1987).*

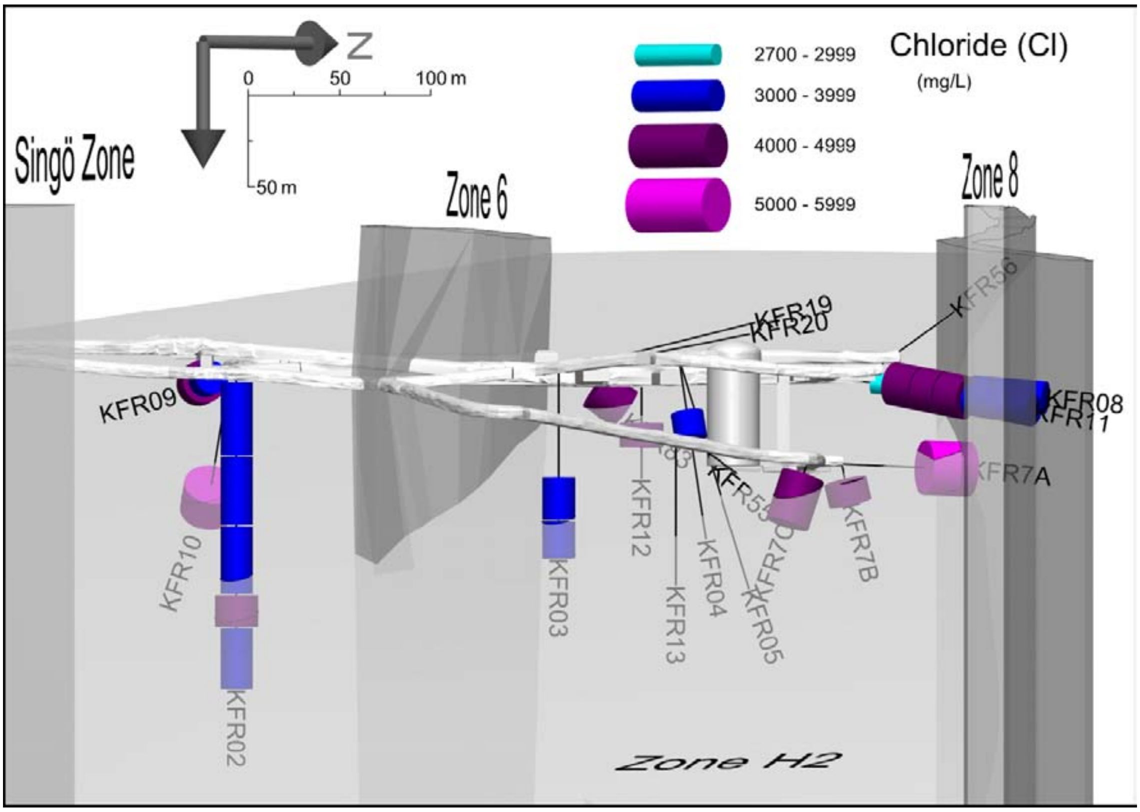


Figure A2-3. *Close view, initial chloride concentrations (1987) through zone H2 and zone 8.*

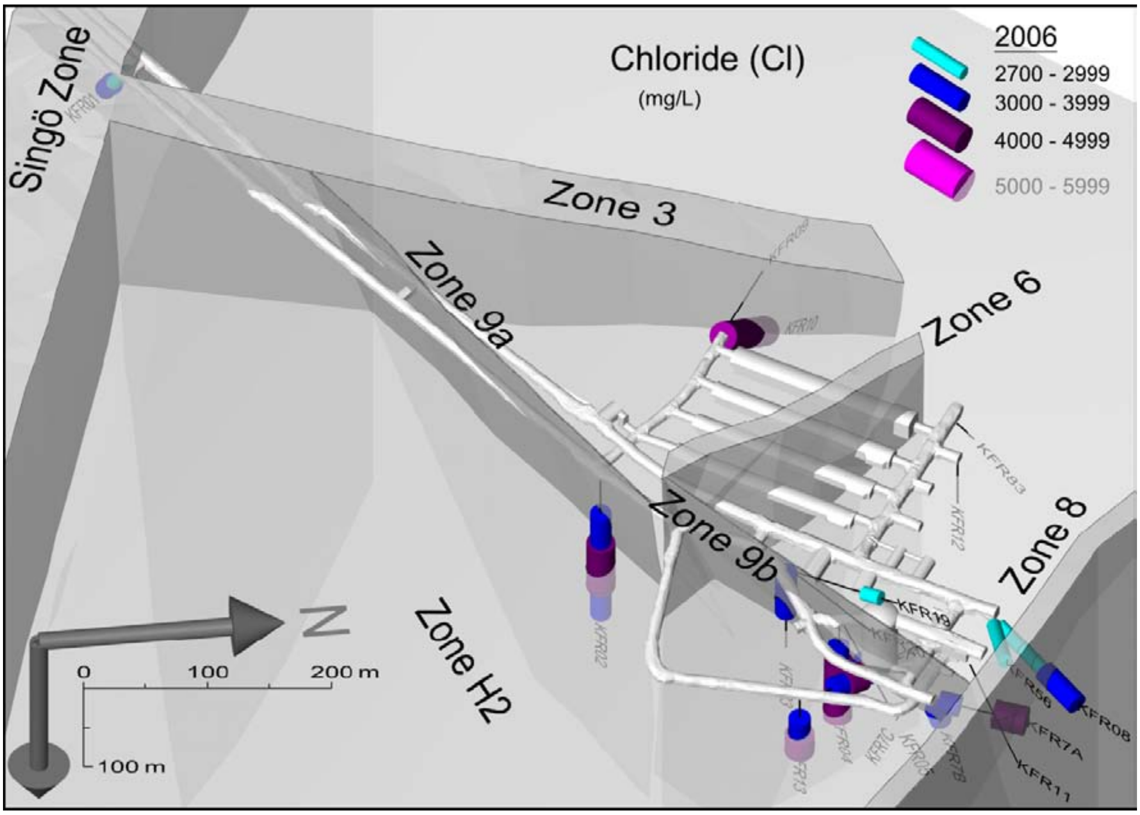


Figure A2-4. *SFR tunnel system, deformation zones and present chloride concentration (2006).*

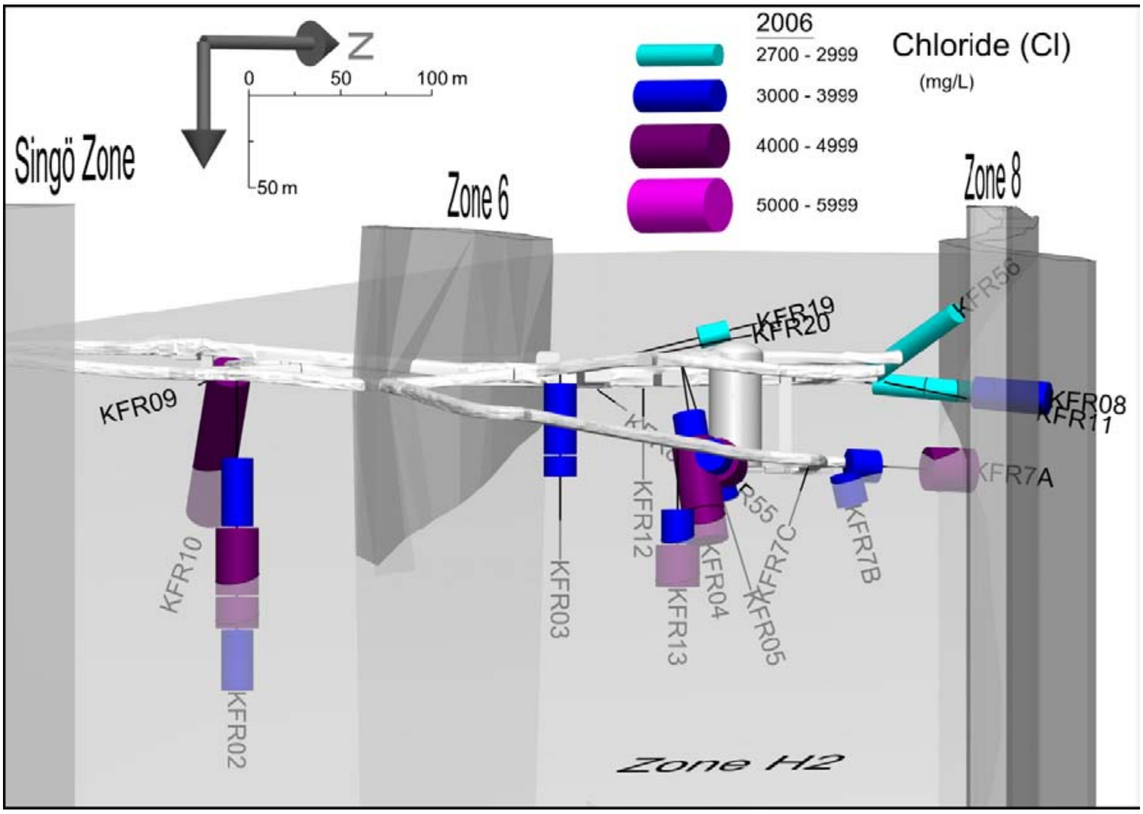


Figure A2-5. *Close view, present chloride concentrations (2006) through zone H2 and zone 8.*

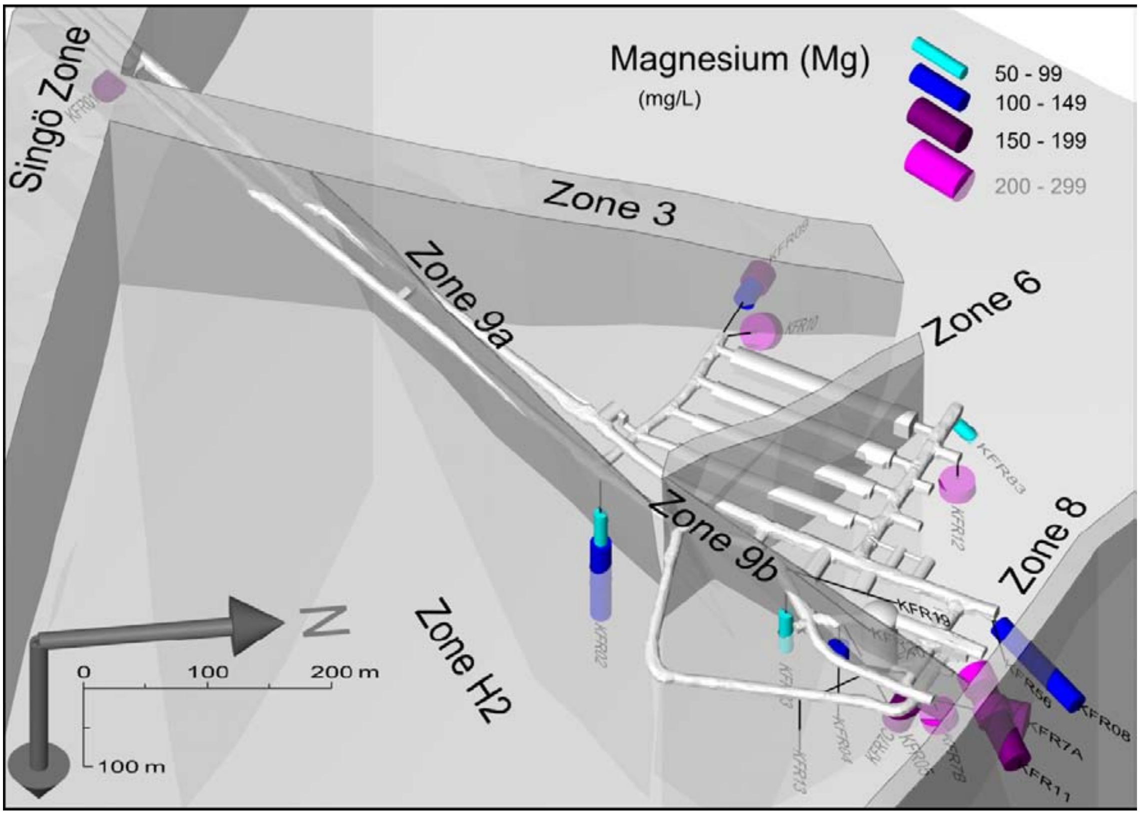


Figure A2-6. SFR tunnel system, deformation zones and initial magnesium concentration (1987).

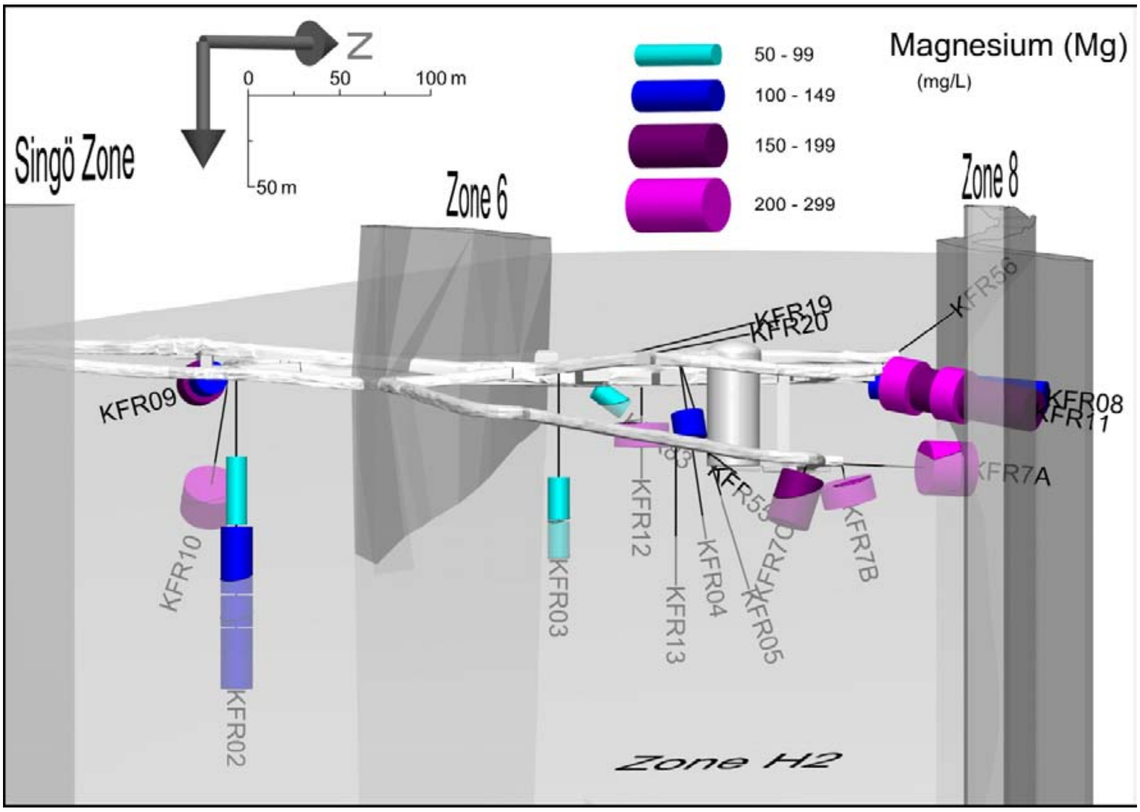


Figure A2-7. Close view, initial magnesium concentrations (1987) through zone H2 and zone 8.

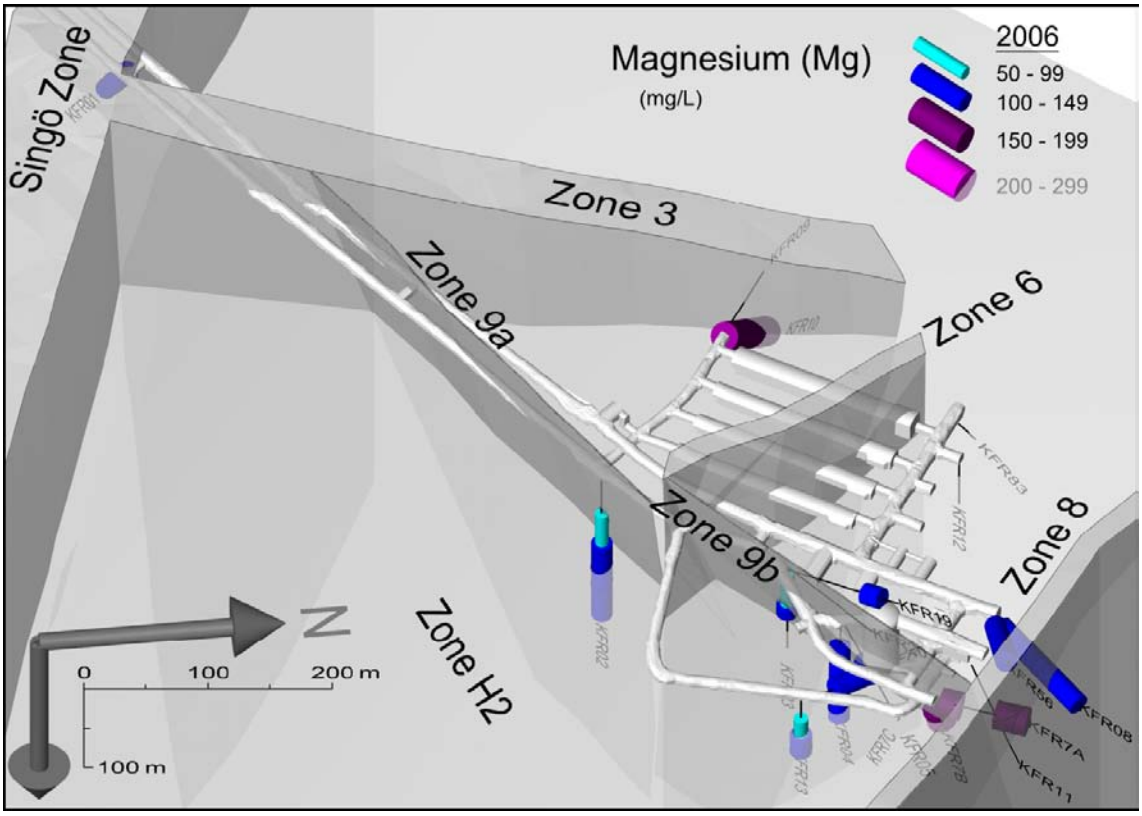


Figure A2-8. *SFR tunnel system, deformation zones and present magnesium concentration (2006).*

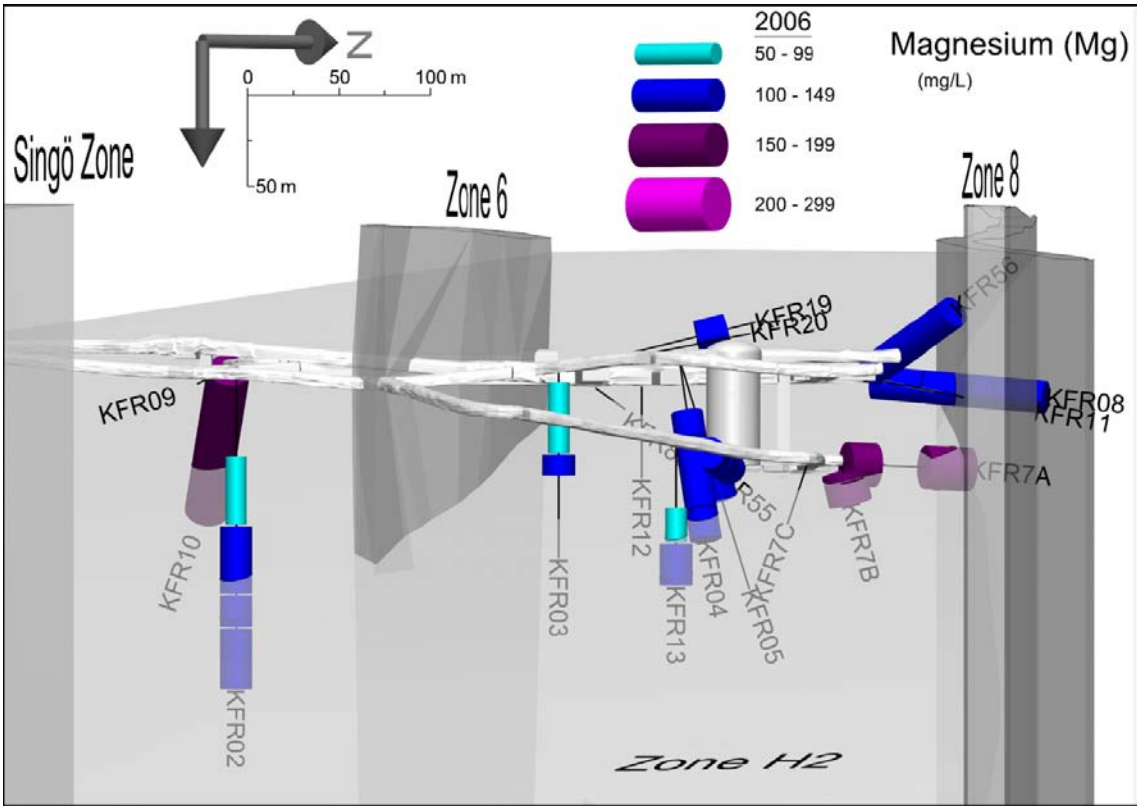


Figure A2-9. *Close view, present magnesium concentrations (2006) through zone H2 and zone 8.*

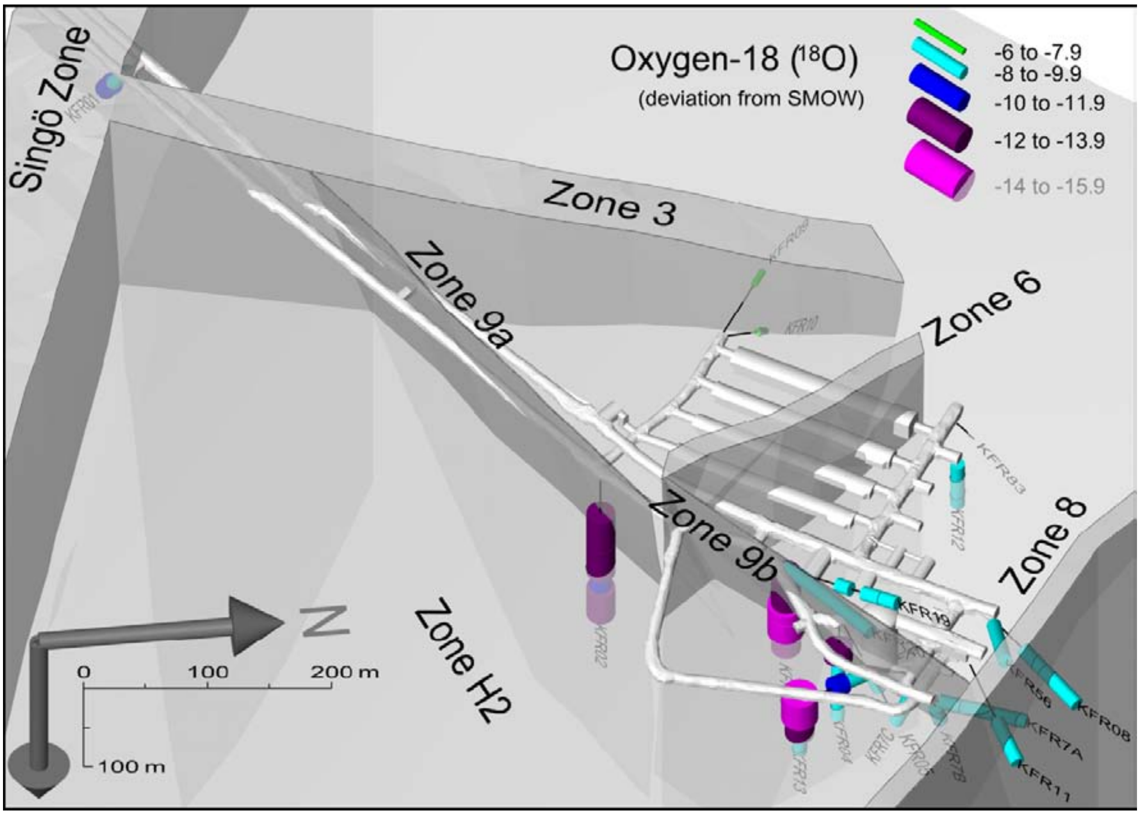


Figure A2-10. SFR tunnel system, deformation zones and early oxygen-18 signature (1995).

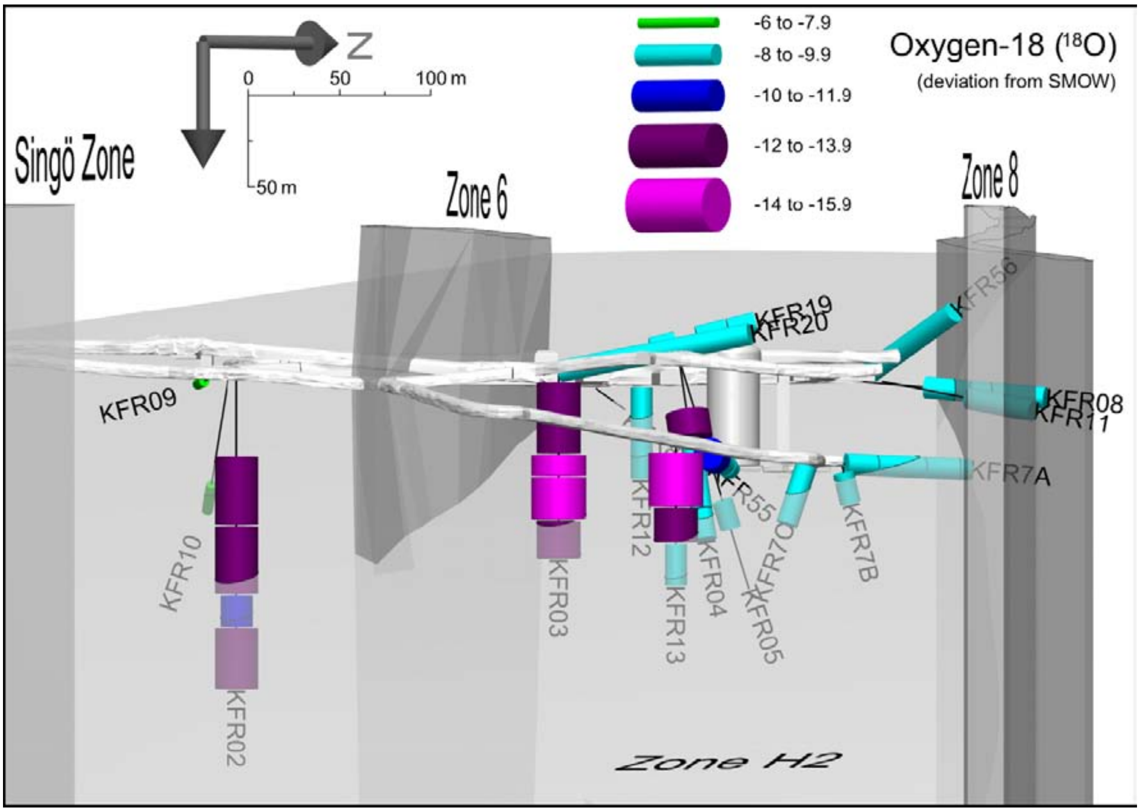


Figure A2-11. Close view, early oxygen-18 signature (1995) through zone H2 and zone 8.

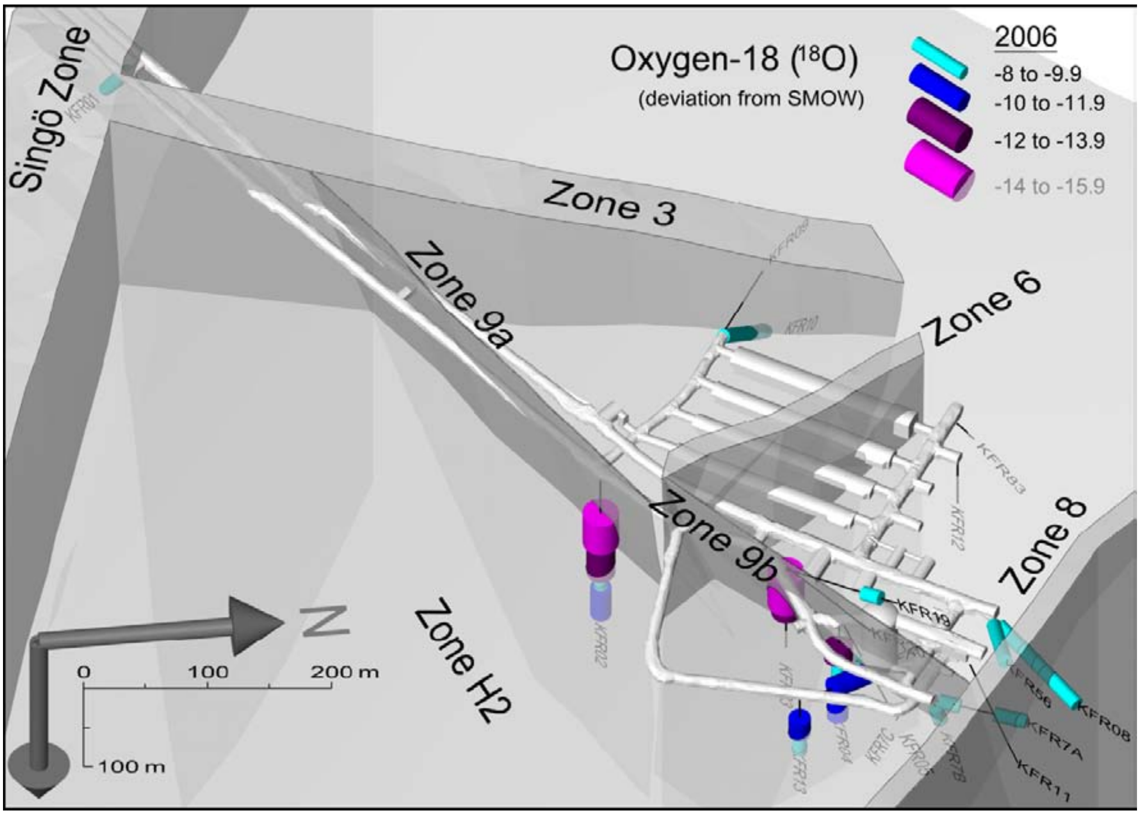


Figure A2-12. *SFR tunnel system, deformation zones and present oxygen-18 signature (2006).*

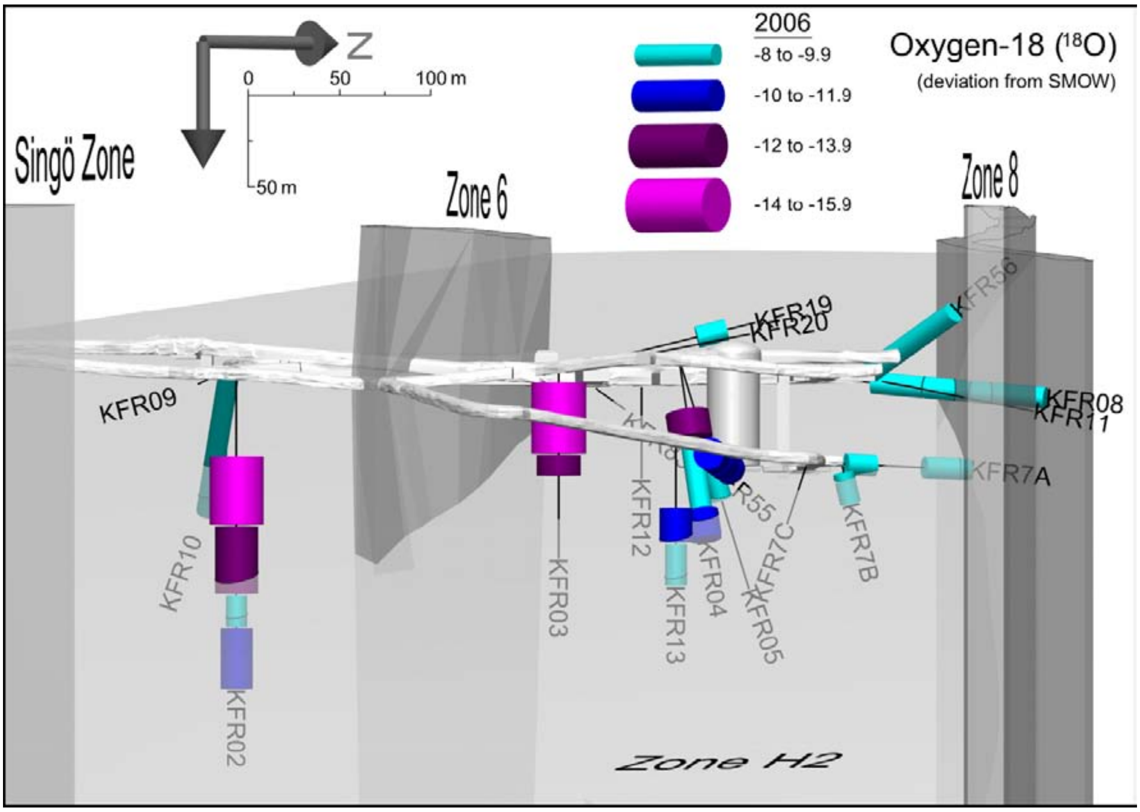


Figure A2-13. *Close view, present oxygen-18 signature (2006) through zone H2 and zone 8.*

Appendix 3

Long term trends

Borehole KFR01; sections 11.0–43.5 (P2) and 44.5–53.4 m.b.l. (P1)

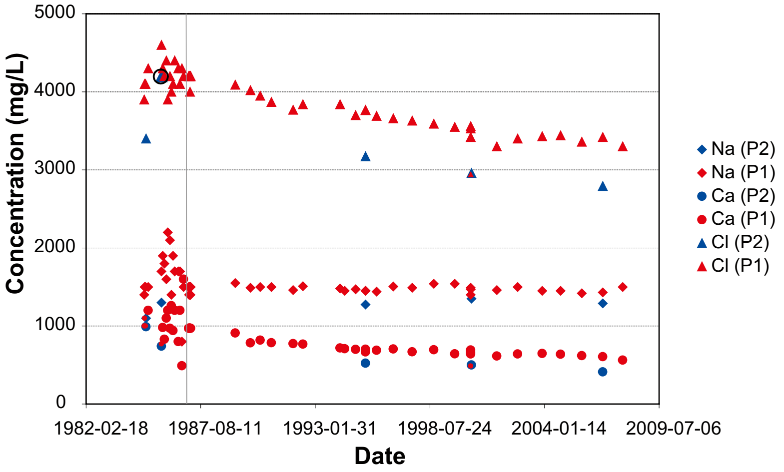


Figure A3-1. *Na, Ca and Cl concentration trends from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable. The marked data point for P2 is verified by EC and used as initial concentration in the 3D-presentation.*

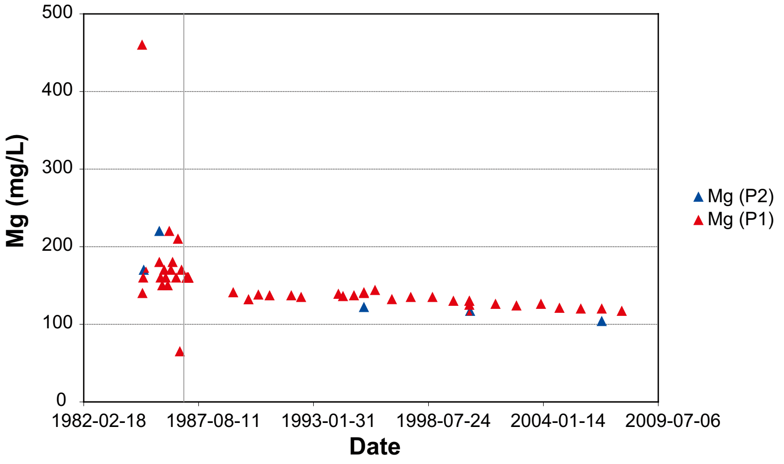


Figure A3-2. *Magnesium trend from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable.*

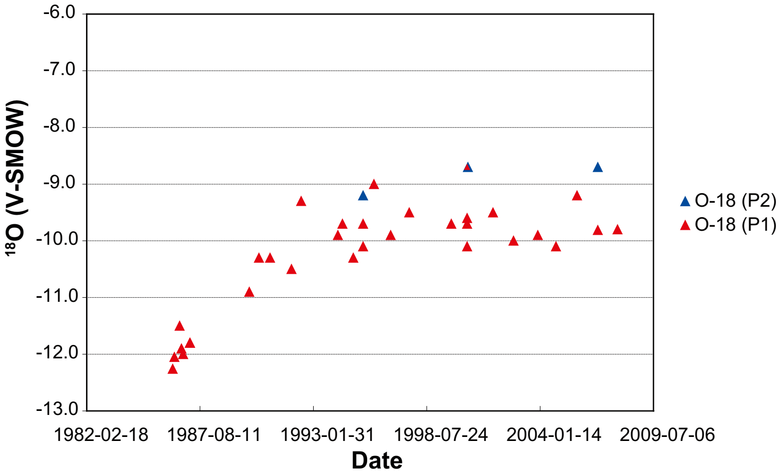


Figure A3-3. *δ ^{18}O (‰ V-SMOW) trend from 1984 to 2007.*

Borehole KFR02; sections 2.0–42.0 (Blind), 43.0–80.0(P4), 81.0–118.0(P3), 119.0–136.0 (P2) and 137.0–170.3 m.b.l. (P1).

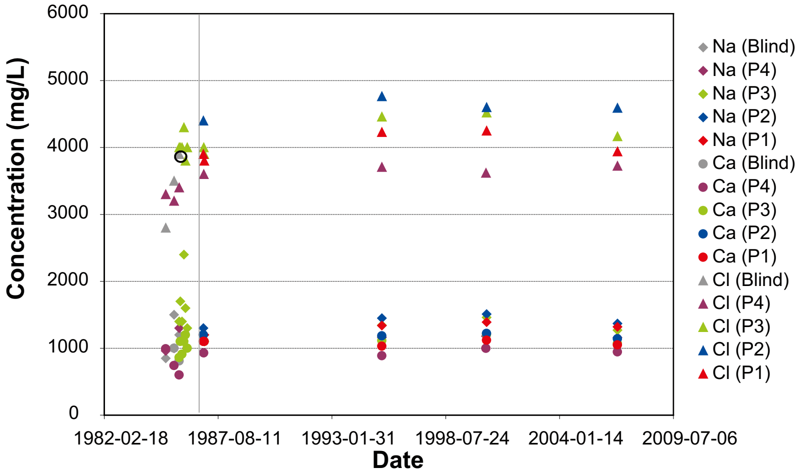


Figure A3-4. *Na,Ca and Cl trends from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable. The marked data point for 'Blind' is verified by EC and used as initial conc. in 3D-figure.*

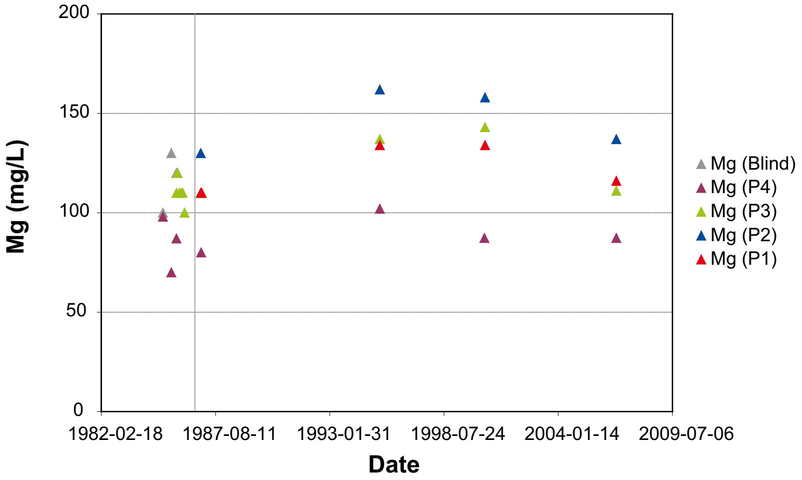


Figure A3-5. *Magnesium trend from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable.*

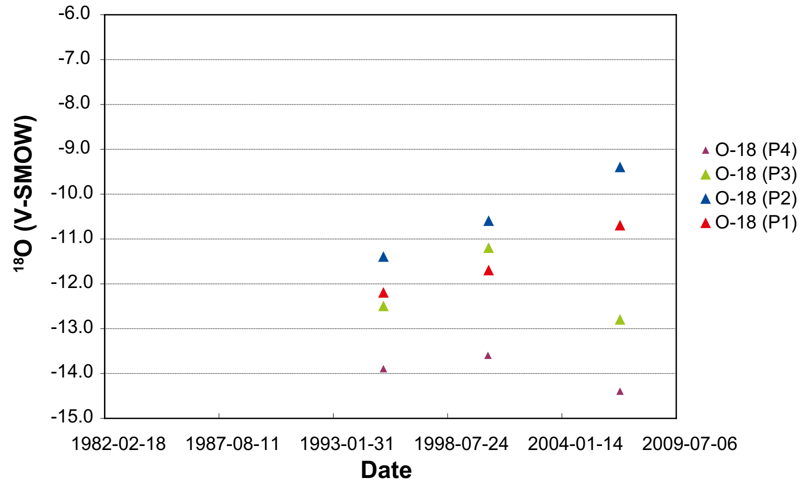


Figure A3-6. *δ ^{18}O (‰ VSMOW) trend from 1995 to 2006.*

Borehole KFR03; sections 5–44 (P4), 45–56 (P3), 57–80 (P2) and 81–106 (P1) m.b.l.

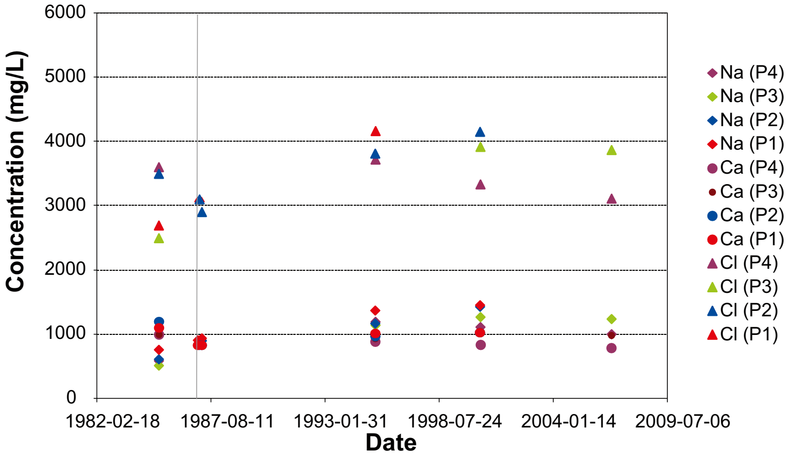


Figure A3-7. *Na, Ca and Cl trends from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable.*

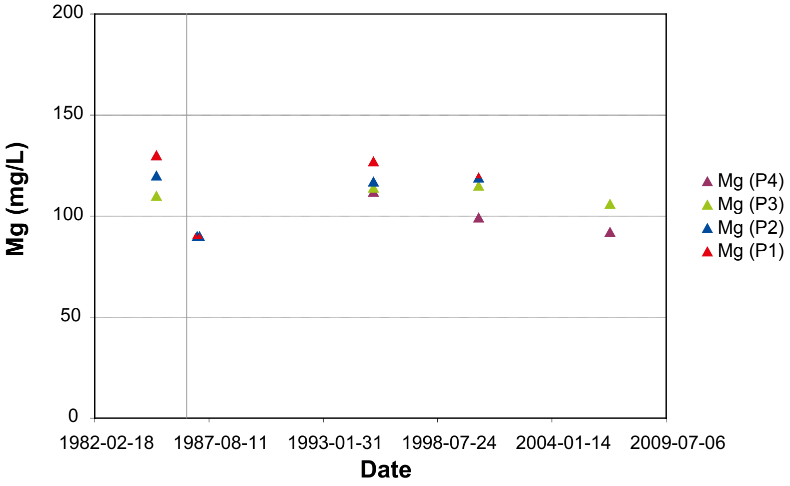


Figure A3-8. *Magnesium trend from 1984 to 2007. Data before Nov. 1986 (vertical .line) are unreliable.*

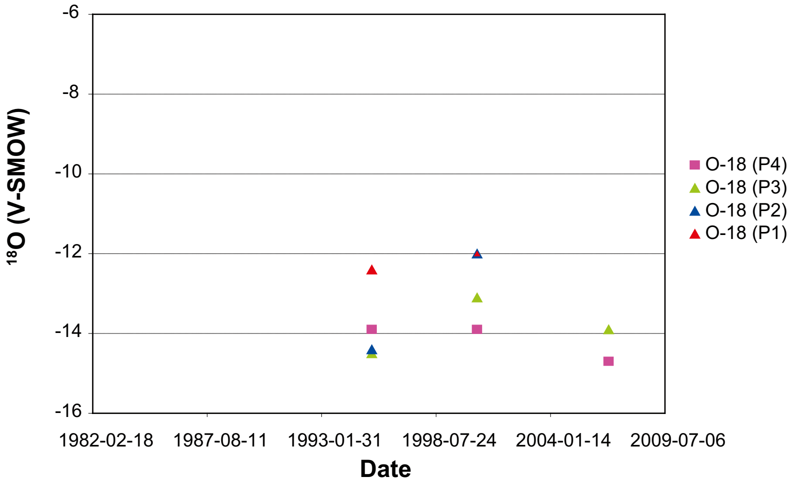


Figure A3-9. *δ ^{18}O (‰ VSMOW) trend from 1995 to 2006.*

KFR04; sections 28–43 (P3), 44–83 (P2) and 84–106 (P1) m.b.l.

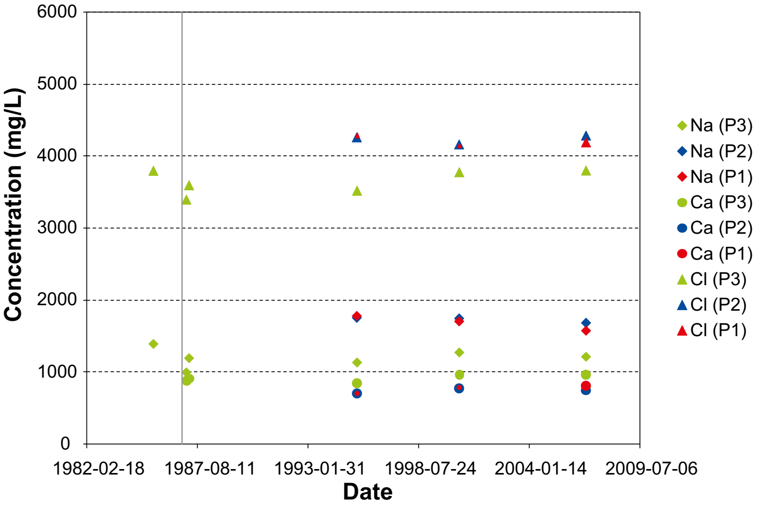


Figure A3-10. *Na, Ca and Cl trends from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable.*

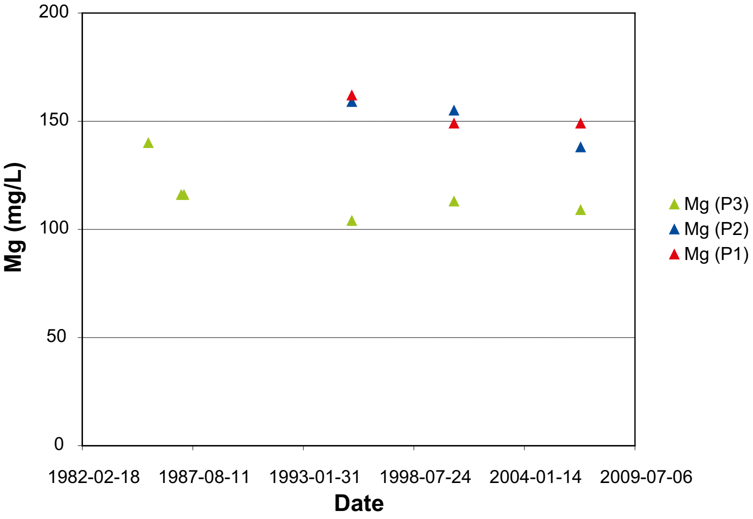


Figure A3-11. *Magnesium trend 1984 to 2007. Data before Nov. 1986 (vertical. line) are unreliable.*

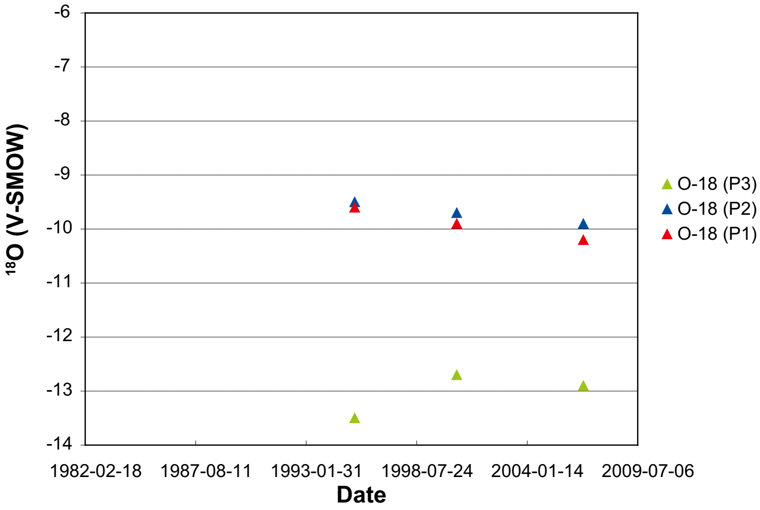


Figure A3-12. *δ ^{18}O (‰ VSMOW) trend from 1995 to 2006.*

KFR08; sections 6–35 (P3), 36–62 (P2) and 63–104 (P1) m.b.l.

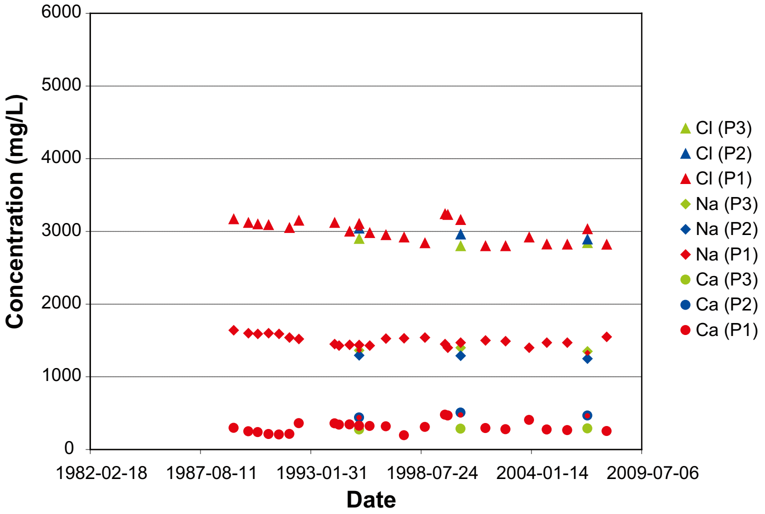


Figure A3-13. *Na,Ca and Cl trends from 1989 to 2007.*

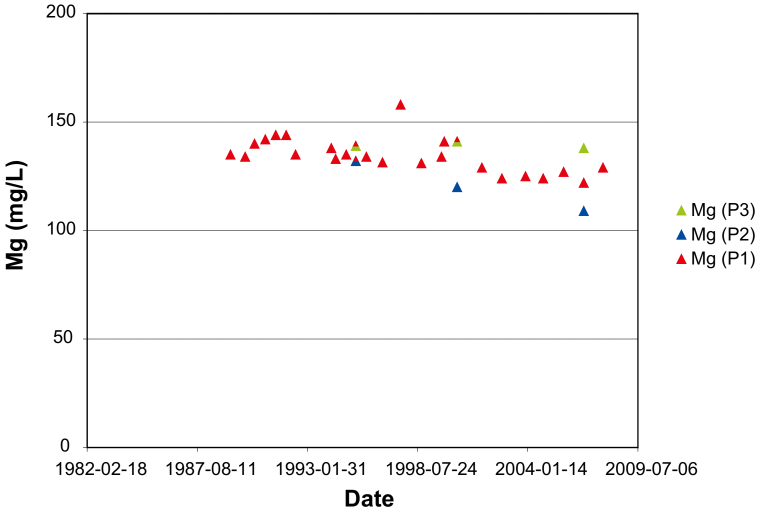


Figure A3-14. *Magnesium trend from 1989 to 2007.*

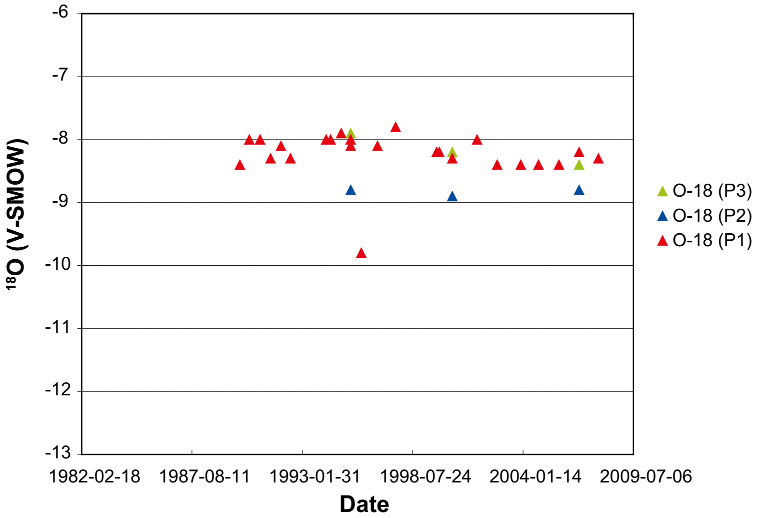


Figure A3-15. *$\delta^{18}O$ (‰ VSMOW) trend from 1989 to 2007.*

KFR09; sections 0–80.2 (entire), 43–62 (P2) and 63–80.2 (P1) m.b.l.

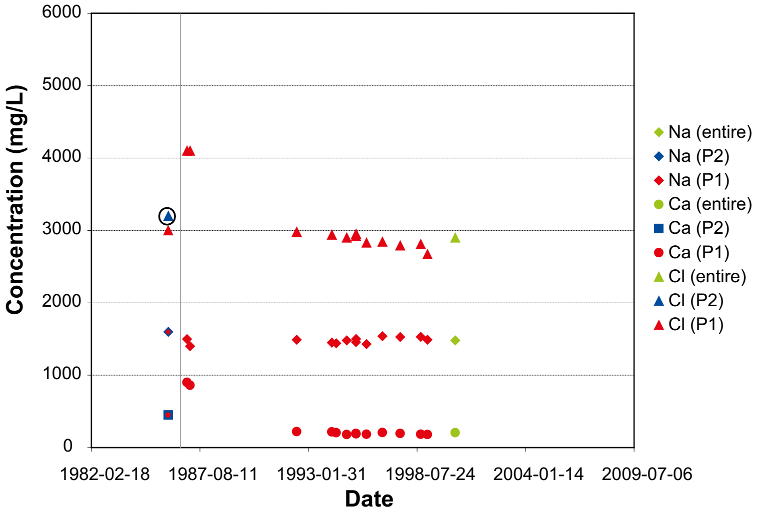


Figure A3-16. *Na,Ca and Cl trends from 1986 to 1999. Data before Nov. 1986 (vertical line) are unreliable. The marked Cl data point for P2 is verified by EC and used as initial conc. in the 3D-figure.*

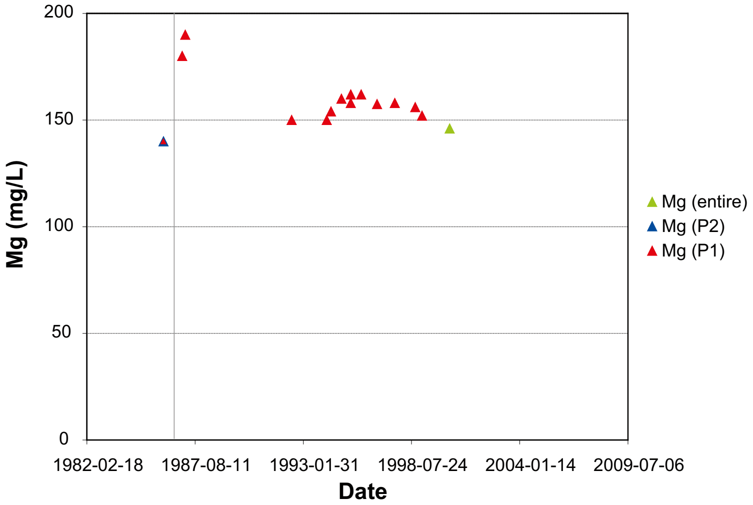


Figure A3-17. *Magnesium trend from 1986 to 1999.*

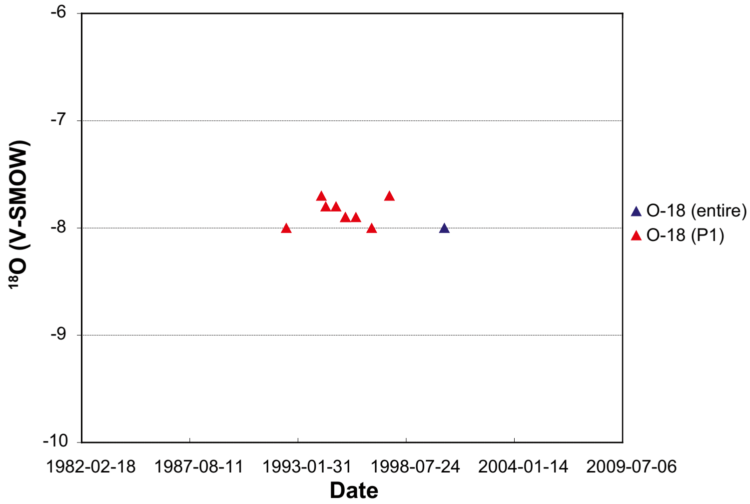


Figure A3-18. *δ^{18}O (‰ VSMOW) trend from 1992 to 1997.*

Borehole KFR10, section 87–107.3 m.b.l (P1) and entire borehole

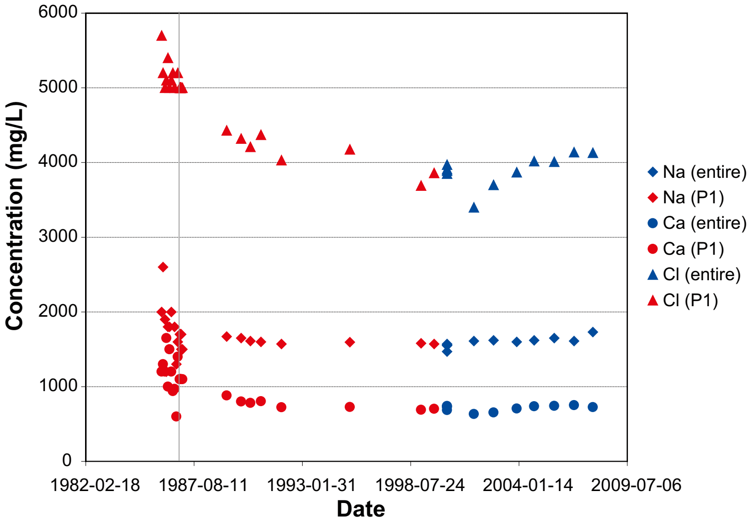


Figure A3-19. *Na,Ca and Cl trends from 1986 to 1999. Data before Nov. 1986 (vertical line) are unreliable.*

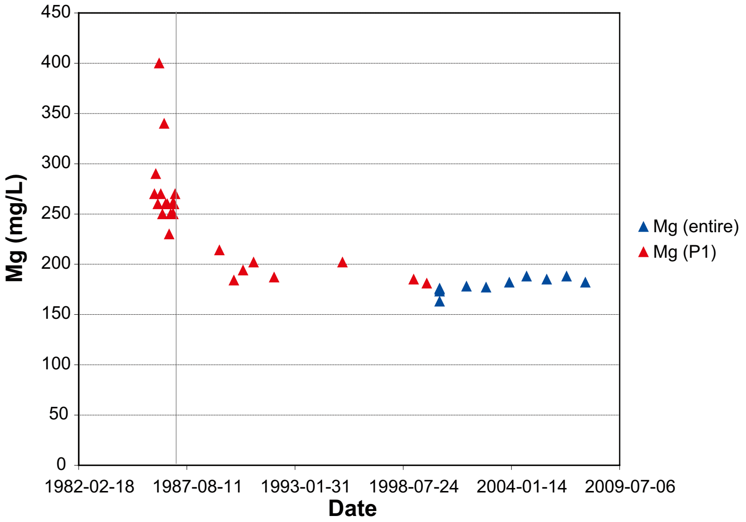


Figure A3-20. *Magnesium trend from 1986 to 1999.*

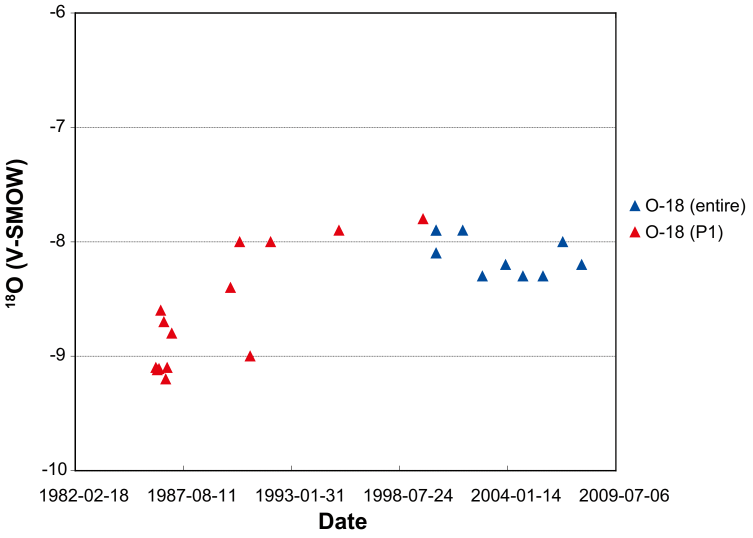


Figure A3-21. *$\delta^{18}O$ (‰ VSMOW) trend from 1992 to 1997.*

Borehole KFR11; sections 7–24 (P4), 25–39 (P3), 40–55 (P2) and 56–98.1 (P1) m.b.l.

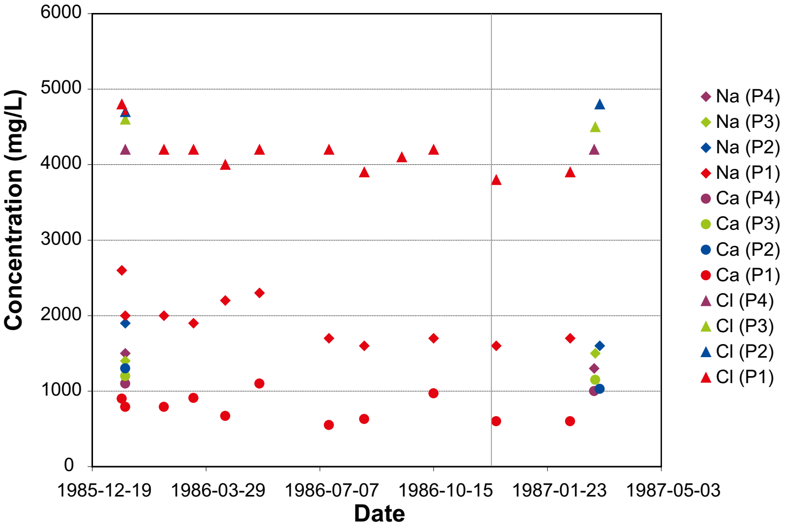


Figure A3-22. *Na,Ca and Cl trends from 1986 and 1987. Data before Nov. 1986 (vertical line) are unreliable.*

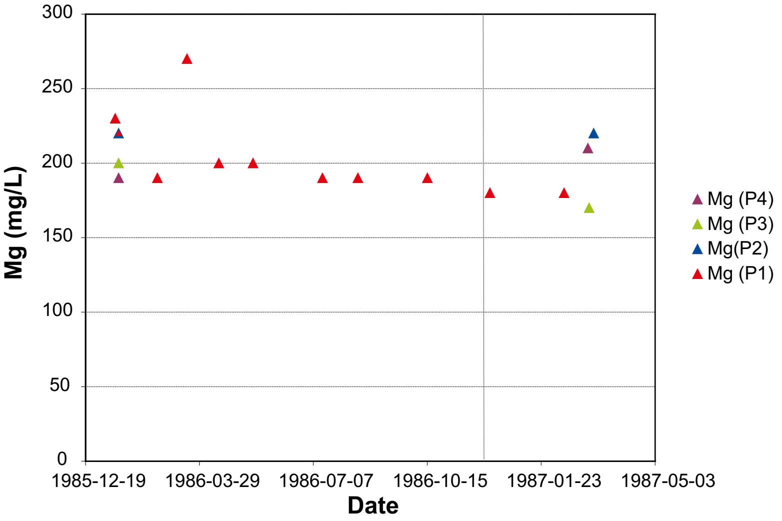


Figure A3-23. *Magnesium trend from 1986 and 1987.*

Borehole KFR7A; sections 2–19 (P3), 20–47 (P2) and 48–74.7 (P1) m.b.l.

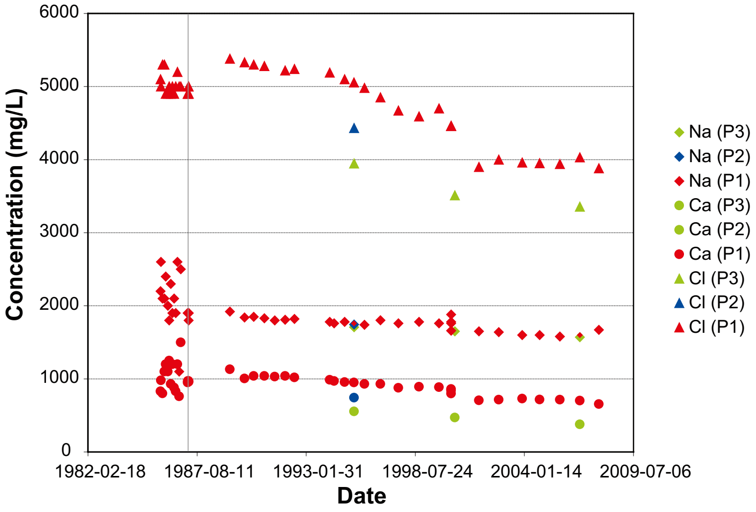


Figure A3-24. Na Ca and Cl concentration trends from 1984 to 2007. Data before Nov. 1986 (vertical line) are unreliable.

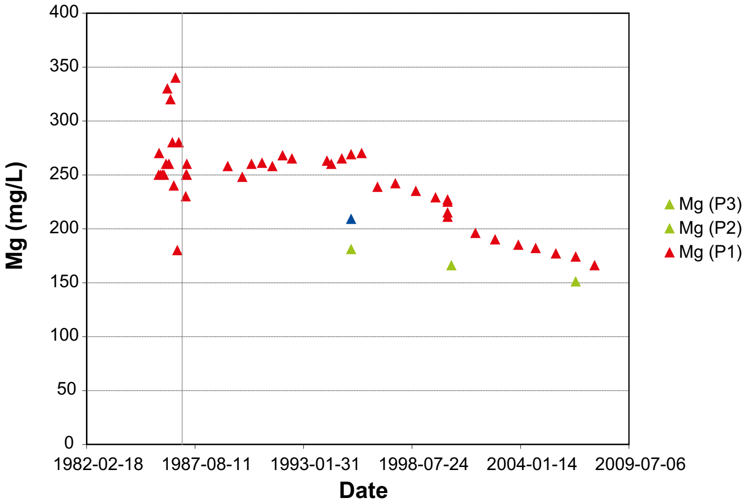


Figure A3-25. Magnesium trend from 1986 to 1999.

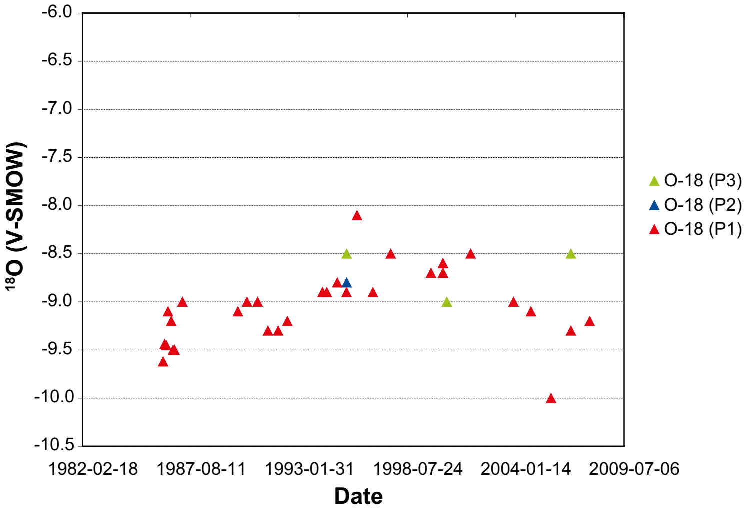


Figure A3-26. δ ^{18}O (‰ VSMOW) trend from 1986 to 2007.

Borehole KFR7B; sections 4–7.6 (P2) and 8.6–21.1 (P1) m.b.l.

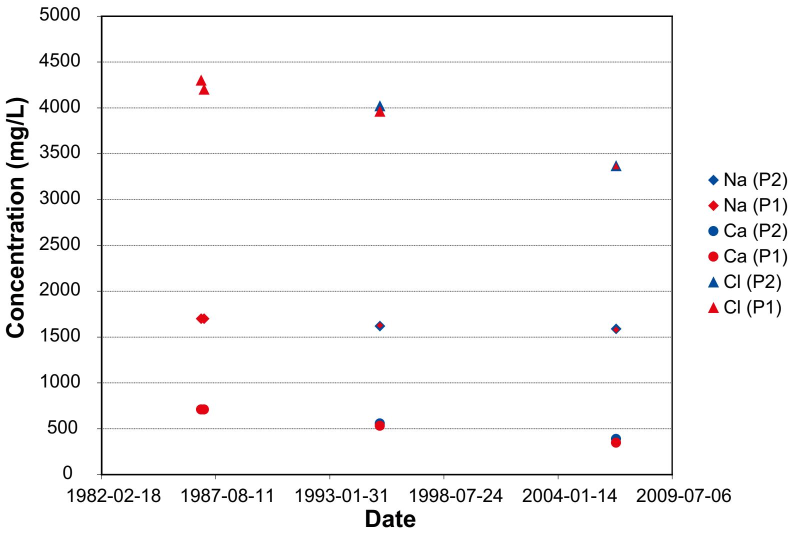


Figure A3-27. *Na,Ca and Cl concentration trends from 1986 to 2007.*

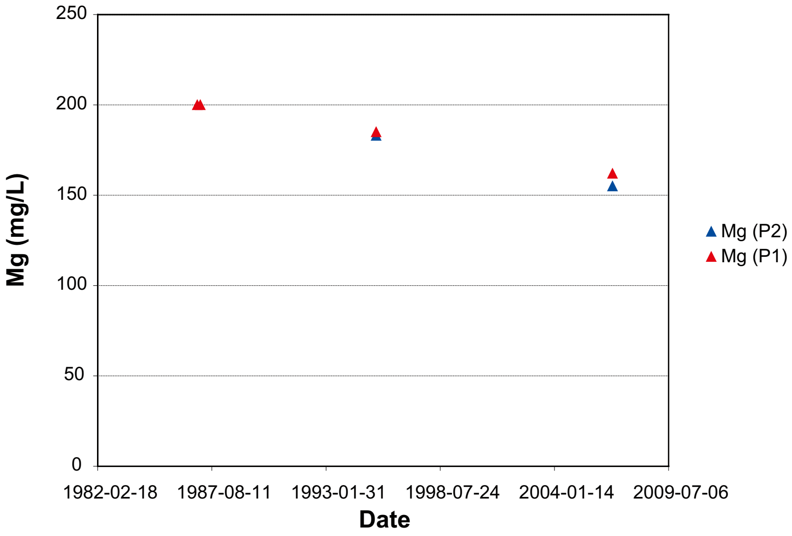
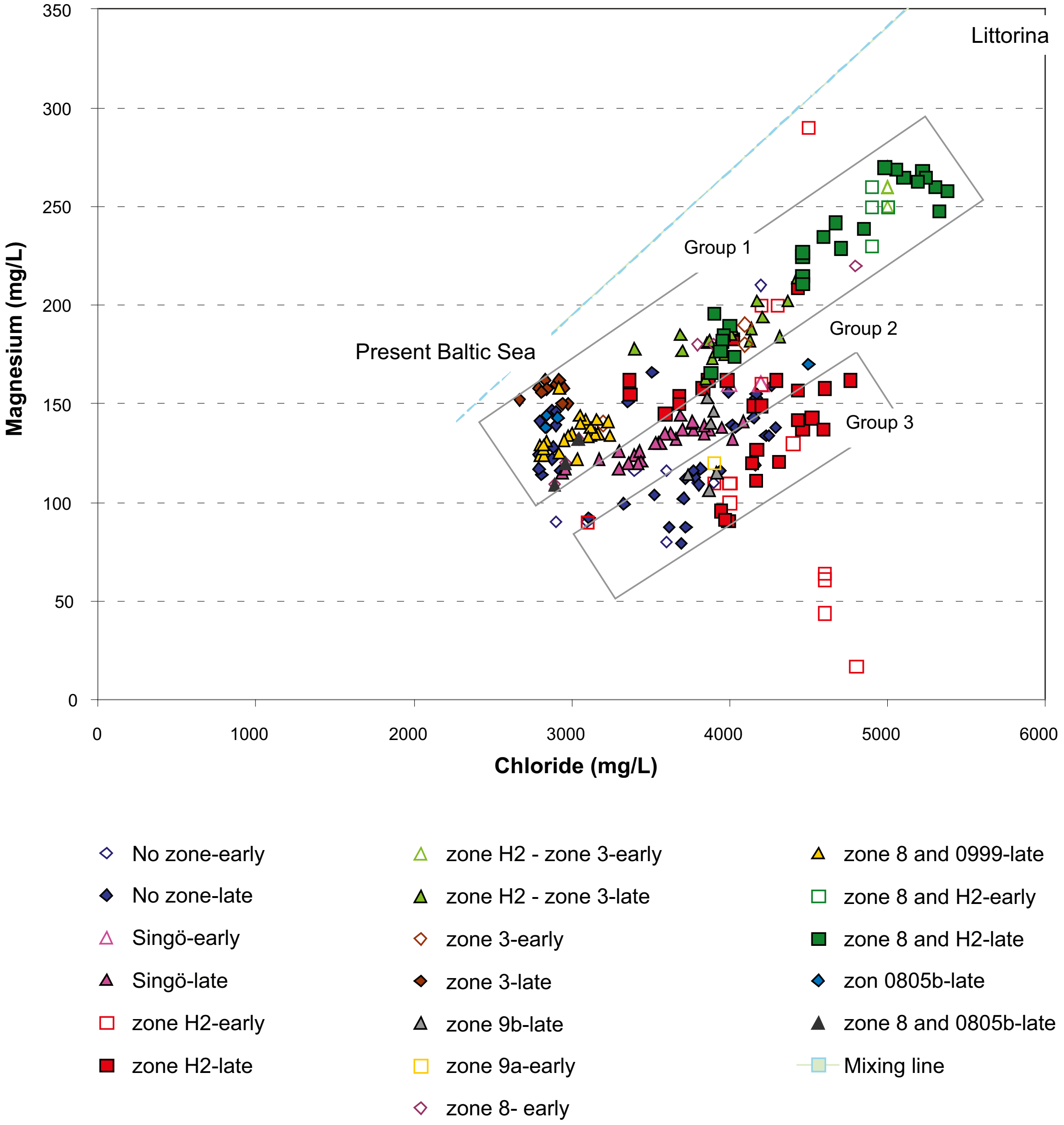
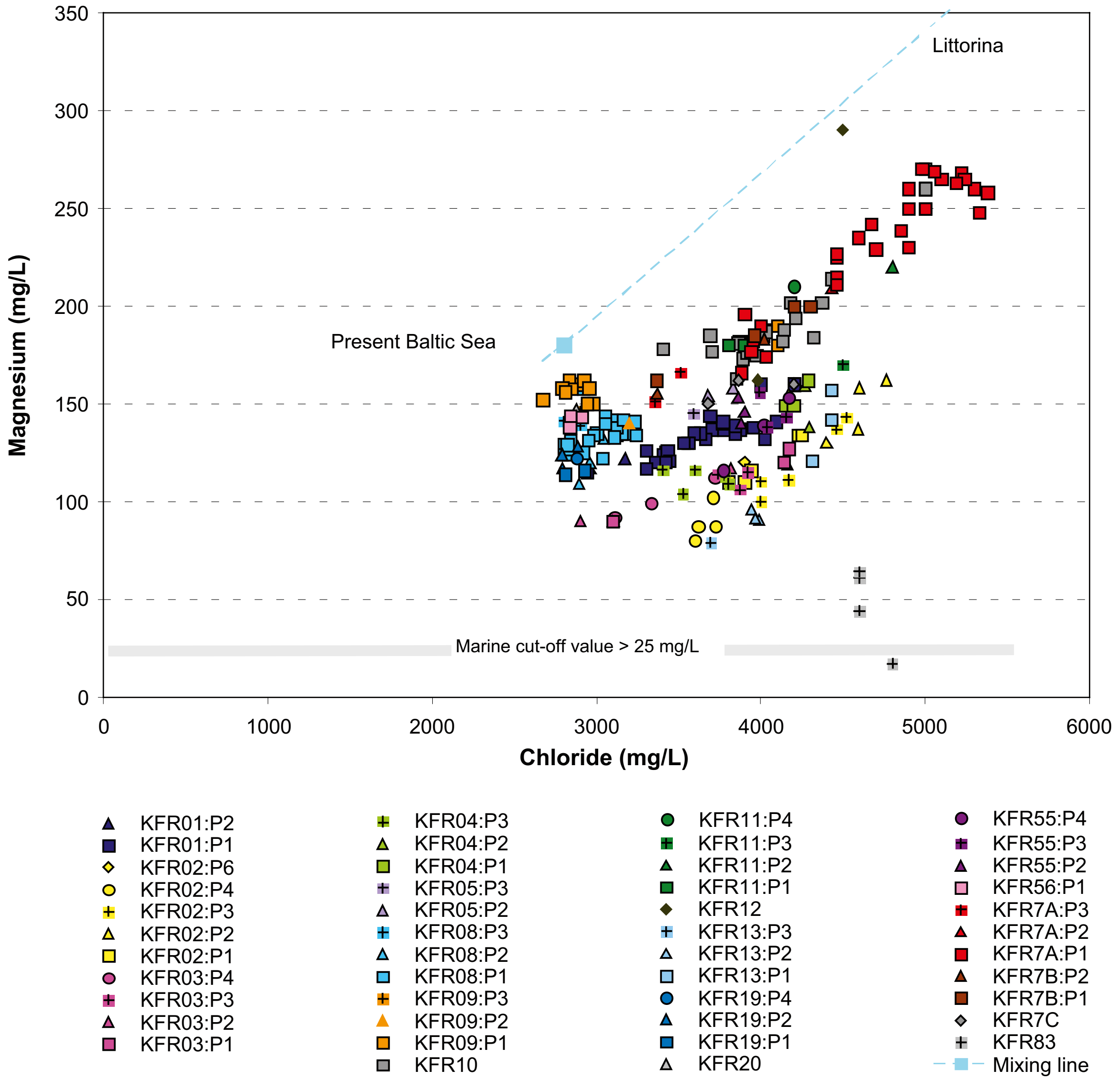


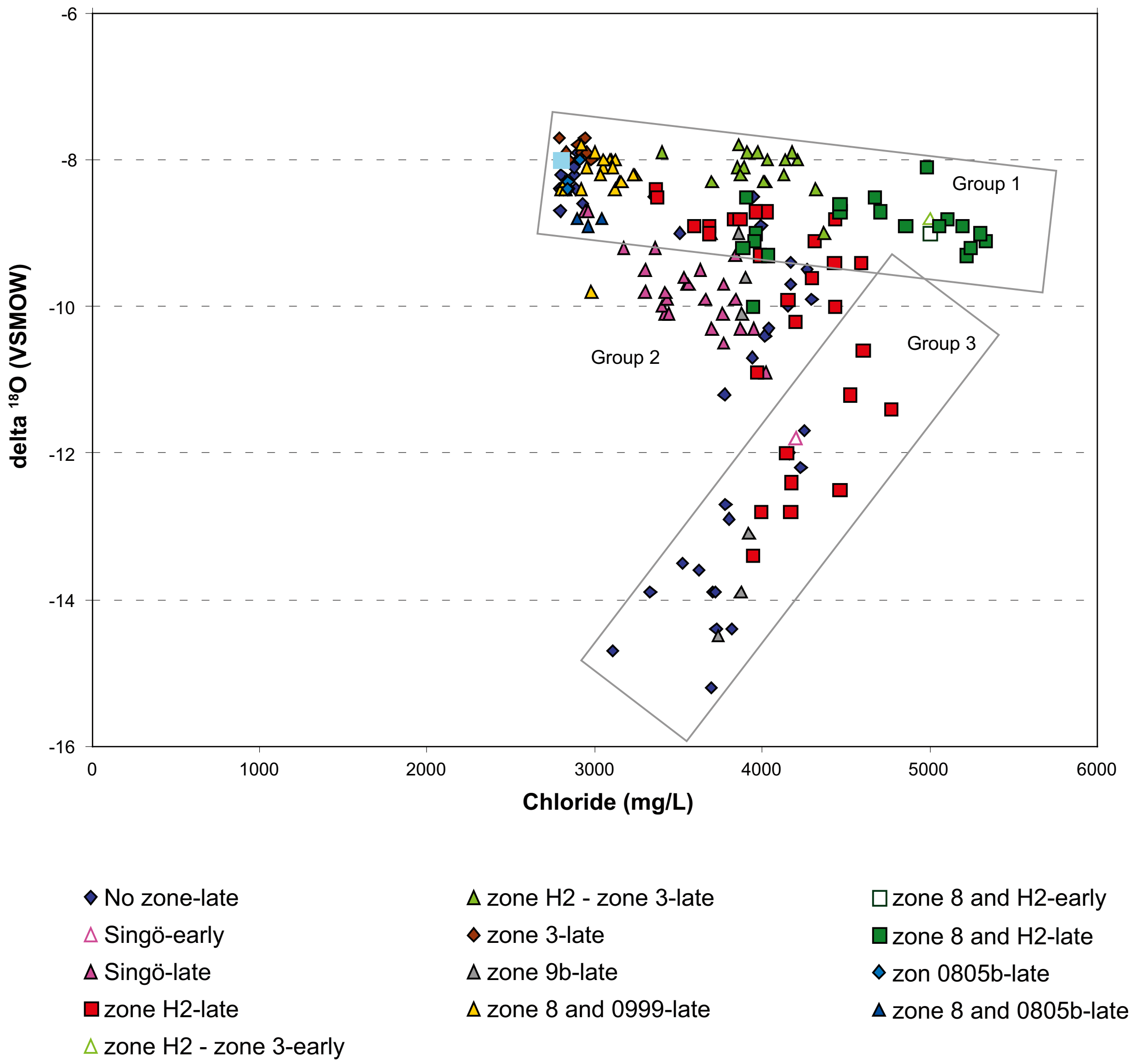
Figure A3-28. *Magnesium trend from 1986 to 1999.*

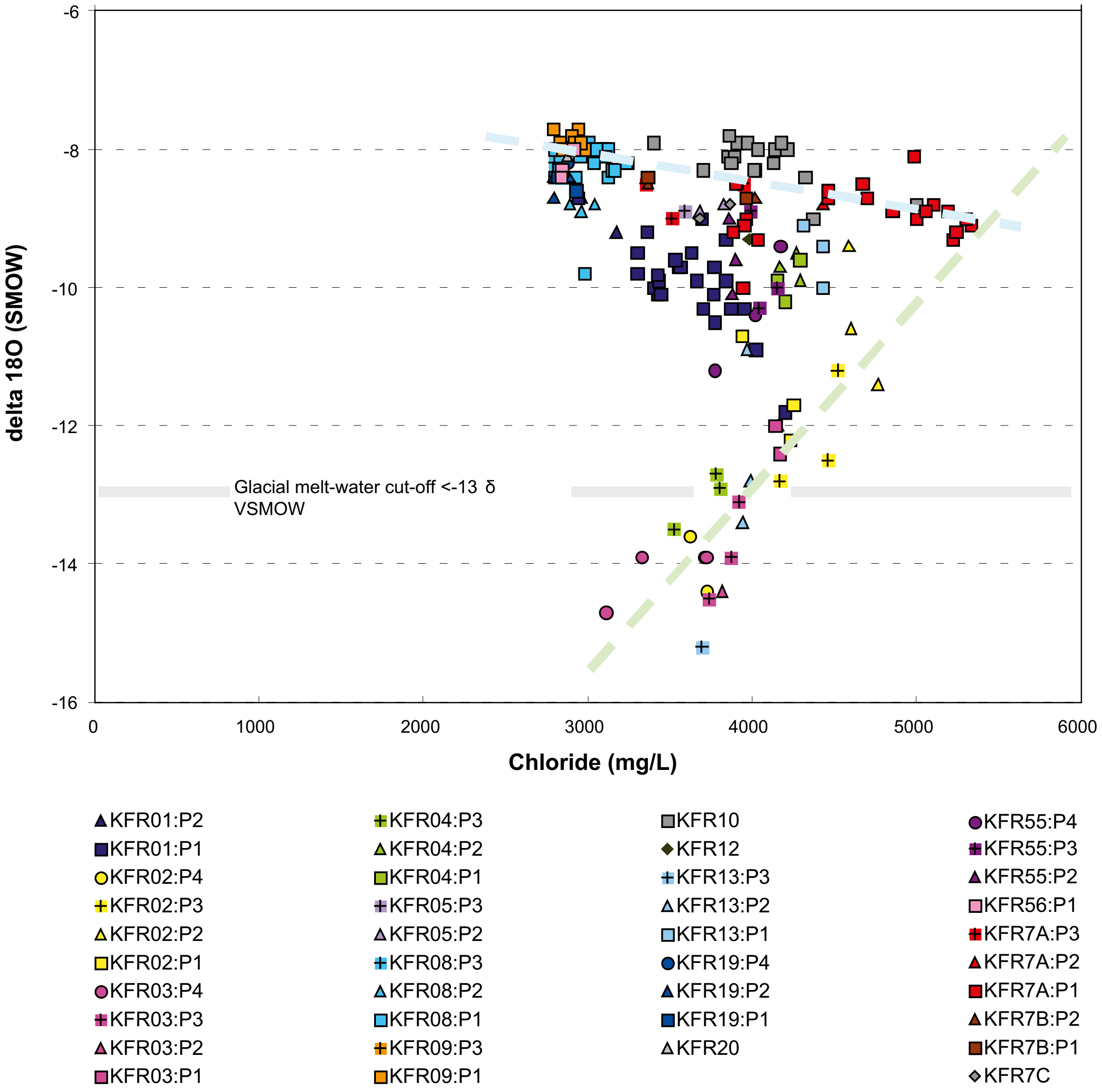
Appendix 4

Magnesium and δ^{18}O versus chloride concentration in x/y scatter plots


Magnesium (mg/L)
350
300
250
200
150
100
50
0
Chloride (mg/L)
0
1000
2000
3000
4000
5000
6000
Littorina
Group 1
Group 2
Group 3
Present Baltic Sea
No zone-early
No zone-late
Singö-early
Singö-late
zone H2-early
zone H2-late
zone H2 - zone 3-early
zone H2 - zone 3-late
zone 3-early
zone 3-late
zone 9b-late
zone 9a-early
zone 8- early
zone 8 and 0999-late
zone 8 and H2-early
zone 8 and H2-late
zon 0805b-late
zone 8 and 0805b-late
Mixing line


Littorina
Present Baltic Sea
Marine cut-off value > 25 mg/L
Magnesium (mg/L)
Chloride (mg/L)
0
50
100
150
200
250
300
350
0
1000
2000
3000
4000
5000
6000
KFR01:P2
KFR01:P1
KFR02:P6
KFR02:P4
KFR02:P3
KFR02:P2
KFR02:P1
KFR03:P4
KFR03:P3
KFR03:P2
KFR03:P1
KFR04:P3
KFR04:P2
KFR04:P1
KFR05:P3
KFR05:P2
KFR08:P3
KFR08:P2
KFR08:P1
KFR09:P3
KFR09:P2
KFR09:P1
KFR10
KFR11:P4
KFR11:P3
KFR11:P2
KFR11:P1
KFR12
KFR13:P3
KFR13:P2
KFR13:P1
KFR19:P4
KFR19:P2
KFR19:P1
KFR20
KFR55:P4
KFR55:P3
KFR55:P2
KFR56:P1
KFR7A:P3
KFR7A:P2
KFR7A:P1
KFR7B:P2
KFR7B:P1
KFR7C
KFR83
Mixing line


-6
-8
-10
-12
-14
-16
delta ¹⁸O (VSMOW)
0
1000
2000
3000
4000
5000
6000
Chloride (mg/L)
Group 1
Group 2
Group 3
No zone-late
Singö-early
Singö-late
zone H2-late
zone H2 - zone 3-early
zone H2 - zone 3-late
zone 3-late
zone 9b-late
zone 8 and 0999-late
zone 8 and H2-early
zone 8 and H2-late
zon 0805b-late
zone 8 and 0805b-late


delta 18O (SMOW)
-6
-8
-10
-12
-14
-16
0
1000
2000
3000
4000
5000
6000
Chloride (mg/L)
Glacial melt-water cut-off <-13 δ VSMOW
KFR01:P2
KFR01:P1
KFR02:P4
KFR02:P3
KFR02:P2
KFR02:P1
KFR03:P4
KFR03:P3
KFR03:P2
KFR03:P1
KFR04:P3
KFR04:P2
KFR04:P1
KFR05:P3
KFR05:P2
KFR08:P3
KFR08:P2
KFR08:P1
KFR09:P3
KFR09:P1
KFR10
KFR12
KFR13:P3
KFR13:P2
KFR13:P1
KFR19:P4
KFR19:P2
KFR19:P1
KFR20
KFR55:P4
KFR55:P3
KFR55:P2
KFR56:P1
KFR7A:P3
KFR7A:P2
KFR7A:P1
KFR7B:P2
KFR7B:P1
KFR7C

Appendix 5

Depth trends (Na, Ca, Mg, HCO_3, Cl and SO_4)

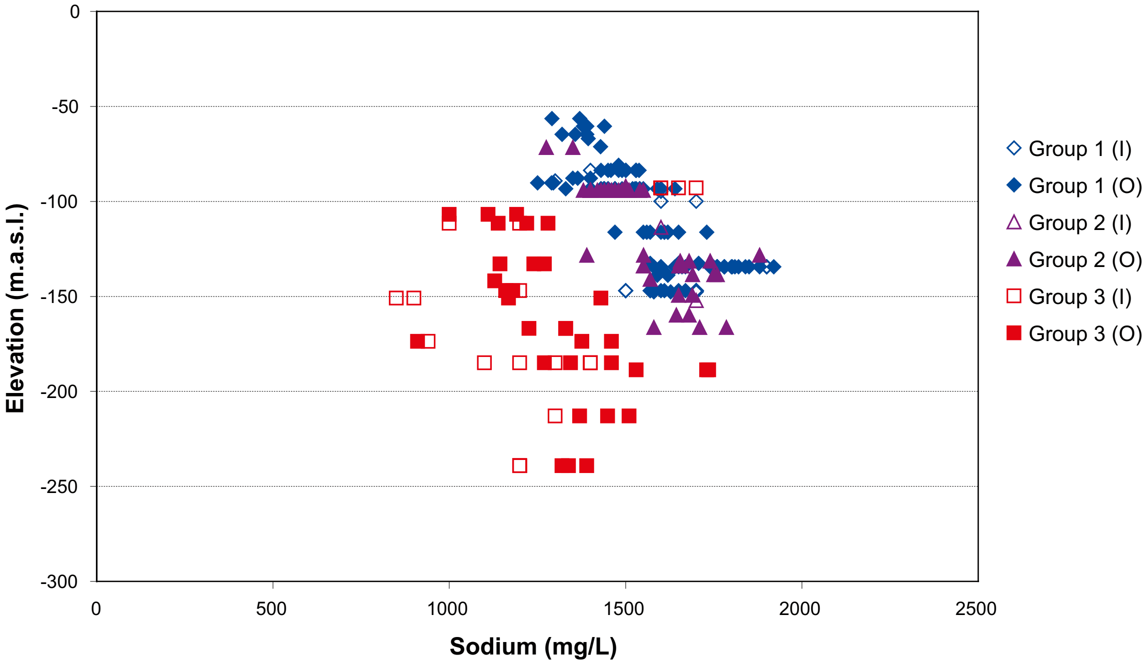


Figure A5-1. *Sodium concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*

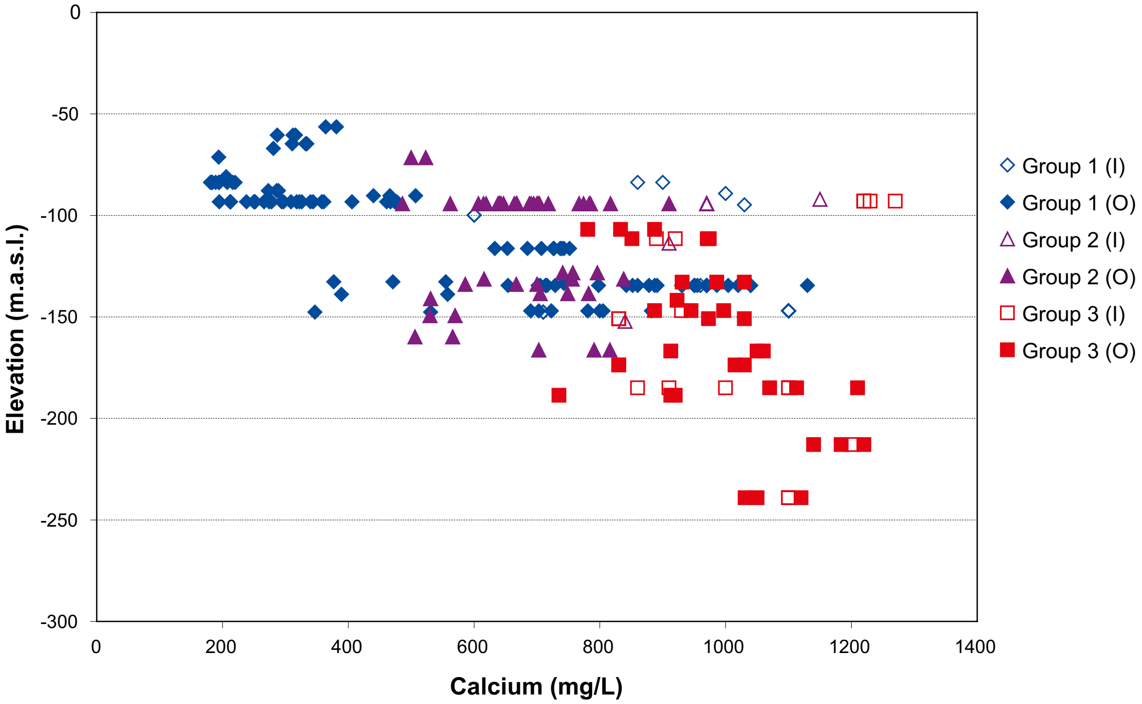


Figure A5-2. *Calcium concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*

Depth trends, Na, Ca, Mg, HCO_3, Cl and SO_4 concentrations

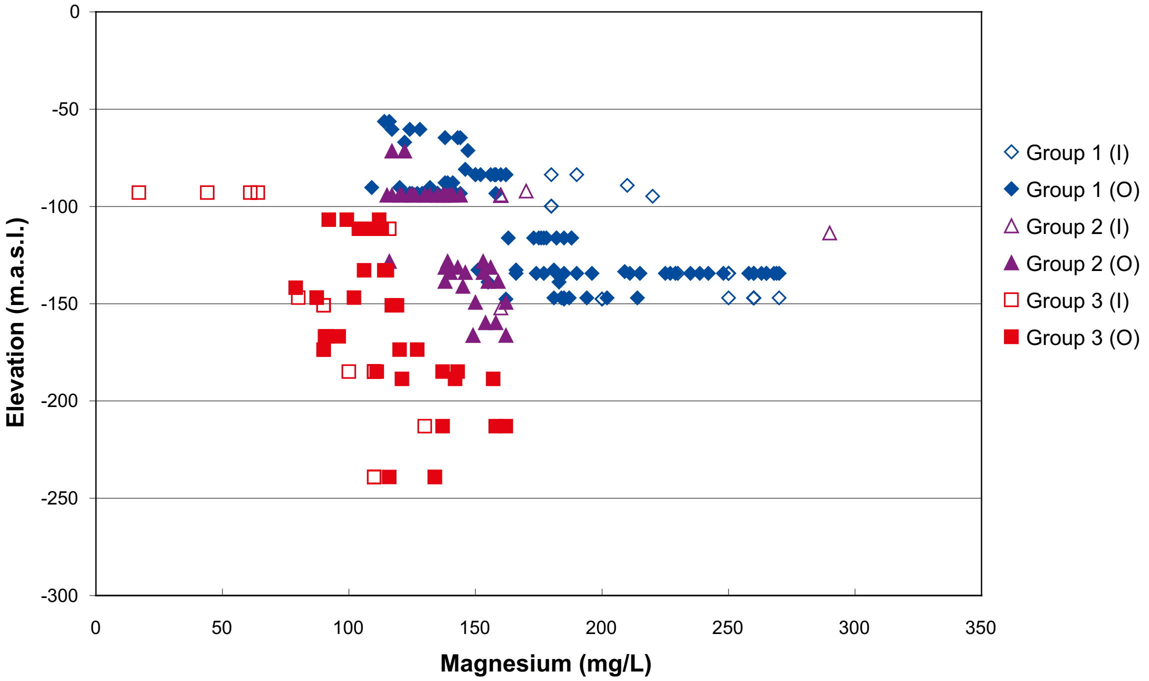


Figure A5-3. *Magnesium concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*

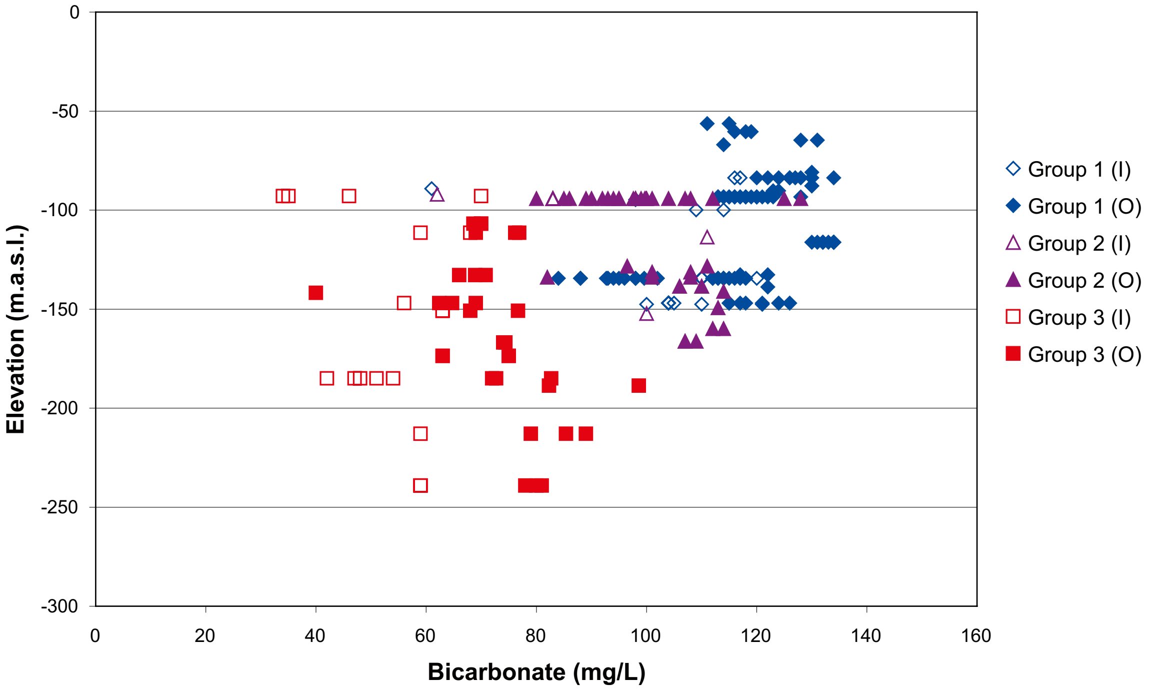


Figure A5-4. *Bicarbonate concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*

Depth trends, Na, Ca, Mg, HCO_3, Cl and SO_4 concentrations

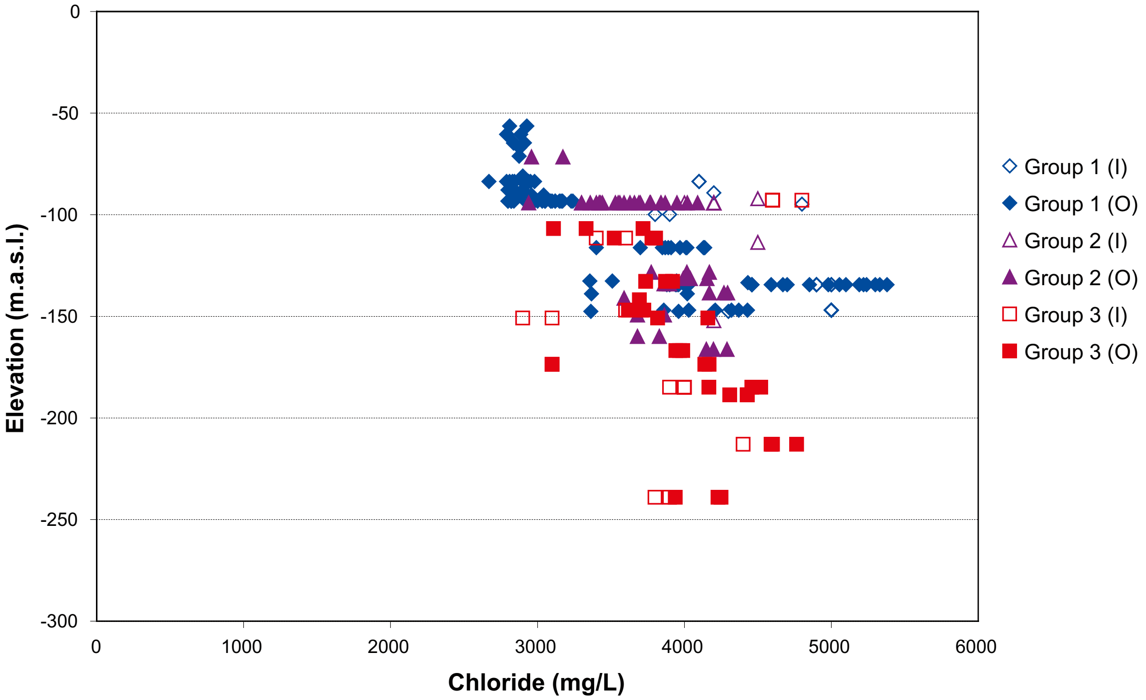


Figure A5-5. *Chloride concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*

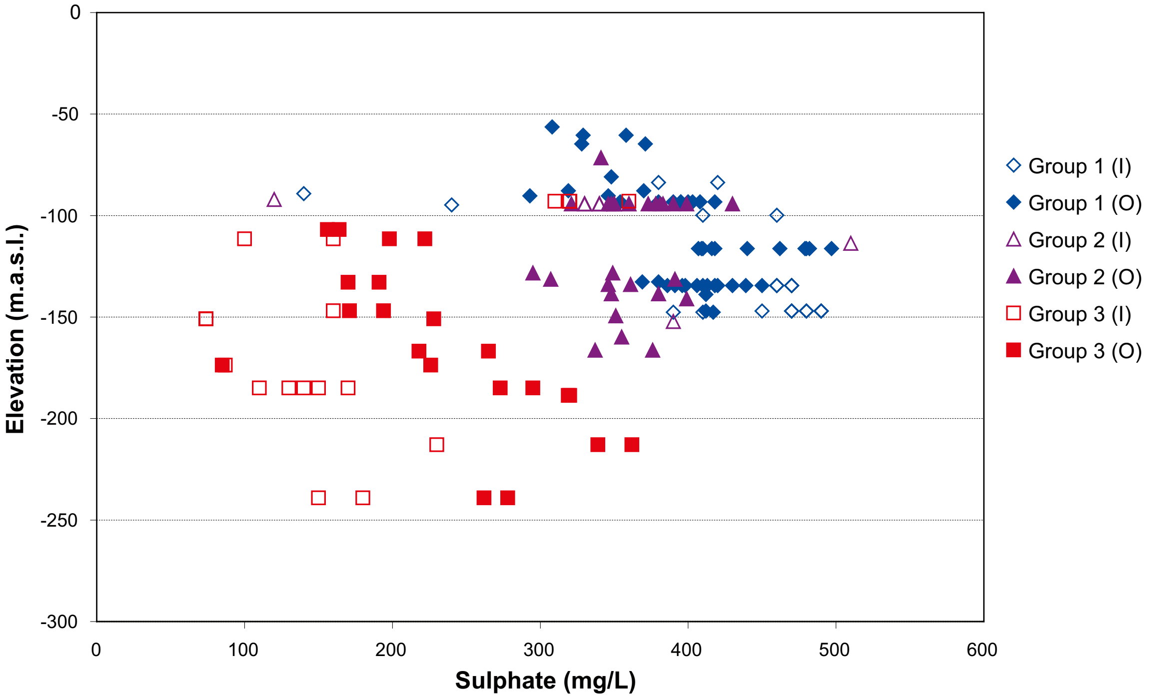


Figure A5-6. *Sulphate concentration versus depth. (I) = initial data and (O) = data obtained during operational phase.*