TECHNICAL
REPORT

95-05

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February 1995

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GROUNDWATER SAMPLING AND CHEMICAL CHARACTERISATION OF THE LAXEMAR DEEP BOREHOLE KLX02

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Information on SKB technical reports from1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40), 1990 (TR 90-46), 1991 (TR 91-64), 1992 (TR 92-46) and 1993 (TR 93-34) is available through SKB.

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1995-02-02

Abstract

English

The Laxemar deep borehole, KLX02 (1705 m depth), located close to the Äspö Hard Rock Laboratory (HRL), has been investigated. Groundwater sampling was conducted on two occasions and using different methods. The first sampling was taken in the open borehole using the so-called Tube sampler; the second sampling carried out using the SKB-packer equipment to isolate pre-determined borehole sections. Groundwater compositions consist of two distinct groupings; one shallow to intermediate *Sodium-Bicarbonate* type [Na(Ca,K):HCO_3-Cl(SO_4)] to a depth of 1000 m, and the other of deep origin, a *Calcium-Chloride type* [Ca-Na(K):Cl-SO_4(Br)], occurring below 1000 m. The deep brines contain up to 46000 mg of Cl per litre. The influence of borehole activities are seen in the tritium data which record significant tritium down to 1000 m, and even to 1420 m. Mixing modelling shows that water from the 1960's is the main source for this tritium. The high tritium values in the 1090-1096.2 m section are due to contamination of 1% shallow water from 1960 and 2% of modern shallow water. The upper 800 m of bedrock at Laxemar lies within a groundwater recharge area; the sub-vertical to moderate angled fracture zones facilitate groundwater circulation to considerable depths, at least to 800 m, thus accounting for some of the low saline brackish groundwaters in these conducting fracture zones. Below 1000 m the system is hydraulically and geochemically "closed" such that highly saline brines exist in a near-stagnant environment.

Swedish

Det 1705 m djupa borrhålet, KLX02, i Laxemar nära Äspölaboratoriet har undersökts. Grundvattnet har vid två tillfällen provtagits med olika metoder. Den första provtagningen utfördes med borrhålet öppet varvid en så kallad slangprovtagare användes. Vid andra vattenprovtagningen användes manschettprovtagare för att avgränsa förutbestämda provtagningssektioner. Grundvattnets sammansättning utgörs av två distinkta grupper. En ytlig till medeldjup vattensort av natriumbikarbonattyp [Na(Ca,K):HCO_3-Cl(SO_4)] som förekommer ner till 1000 m djup och en vattensort med djupt ursprung av kalciumkloridtyp [Ca-Na(K):Cl-SO_4(Br)] som förekommer djupare än 1000 m. Saltvattnet innehåller upp till 46000 mg Cl per liter. Borrhålsaktiviteternas inverkan på vattenkemin påvisas av de höga

tritiumvärdena uppmätta ner till 1000 m och rentav så djupt som 1420 m. Blandningsmodellering visar att vatten från 1960 är den största tritiumkällan. De höga tritumvärdena i sektionen 1090-1096.2 m beror på kontaminering av 1% ytvatten från 1960 och 2% modernt ytvatten. Laxemarberggrundens övre 800 m ligger i grundvattnets inflödesområde. Nästan vertikala sprickzoner främjar grundvattnets omlopp till betydande djup, minst 800 m. Detta förklarar till viss del de bräckta grundvattnen med låg salthalt i dessa vattenledande sprickzoner. Djupare än 1000 m är systemet hydraliskt och geokemiskt "slutet" på så vis att de mycket salta grundvattnen existerar i en nästan stagnant miljö.

Contents

Summary

The Laxemar deep borehole, KLX02, is located close to the Äspö Hard Rock Laboratory (HRL), adjacent to the Baltic coast approximately 350 km south of Stockholm. At 1705 m, KLX02 represents the deepest borehole drilled within the Research and Development programme managed by the Swedish Nuclear Fuel and Waste Management Company (SKB).

The main aims behind locating such a deep borehole at Laxemar are to increase knowledge of rock composition, rock characteristics, groundwater flow paths and groundwater composition at larger depths and in a wider regional context than has been possible within the Äspö project.

In common with Äspö the dominant rock-types comprise, in decreasing order of importance, Småland Granite, Äspö Diorite, Greenstone and Fine-grained Granite. The main fracture filling mineral phases consist of, in decreasing order of frequency: group A (calcite, chlorite), group B (hematite, Fe-oxyhydroxides, epidote, fluorite), and group C (pyrite, magnetite, laumontite/prehnite, gypsum). The underlined fracture minerals are the main types found in the water conducting fractures.

The areal distribution of hydraulic conductivity on Laxemar on the site-specific scale is believed to be heterogeneous, with a significant downward gradient through a series of sub-vertical fractures, perhaps extending down to 500-700 m. Downhole hydraulic tests showed that about 60% of the total discharge is recovered from the upper 250 m of bedrock and about 20% from depths below 500 m. Overall, both the specific storage coefficient and specific transmissivity decrease with depth, and that during pumping the specific storage coefficient is twice that during recovery.

Groundwater sampling was conducted on two occasions and using different methods. The first sampling was taken in the open borehole using the so-called Tube sampler. The second sampling was carried out using the SKB-packer equipment to isolate pre-determined borehole sections. Generally, samples taken with the Tube sampler might be considered of lower quality when compared with the SKB double packer sampling system. Interestingly this is not the case (except for the pH values); comparison with most elements indicate a surprisingly similar character although a somewhat more dilute, i.e. less saline Cl^- concentration, is represented by the waters collected by the Tube sampler. Consequently, these data have been incorporated in the present evaluation.

The groundwater compositions consist of two distinct groupings; one shallow to intermediate *Sodium-Bicarbonate* type

[Na(Ca,K):HCO_3-Cl(SO_4)] to a depth of 1000 m. and the other of deep origin a *Calcium-Chloride type* [Ca-Na(K):Cl-SO_4(Br)] occurring below 1000 m. Two main evolution patterns has been identified by using Principal Component analyses; an assumed *Shallow water - Old Saline water* evolution pattern and a *Baltic Sea - Glacial meltwater* evolution pattern. The KLX02 waters seem to have resulted mainly from the former evolution pattern, i.e. incorporating Modern Shallow, 1960 Shallow and Old Saline water, although an input from the *Baltic Sea - Glacial meltwater* evolution may have caused some influence at depths shallower than 1000 m.

A *Simple Mixing-Mass balance* model has been used to separate the effect on the groundwater from mixing versus reactions. The distance from any observation to the selected six end-members can be calculated directly from a Principal Component plot by using simple trigonometrical functions. The distance is equivalent with the mixing ratios of any observed water in the system. In the samples from the tube sampler a high portion of modern shallow water is seen in the upper part of the borehole (<100 m). At the 100-900 m depth shallow water from the 1960 (high tritium water) and modern shallow water dominates. At the 950 m depth an important portion (20%) of old shallow water occurs. At the deepest section of the borehole (1000-1600 m) glacial meltwater and old saline water dominates. In the samples extracted from the fractures, a similar situation seems to prevail although the portion of old shallow water seems to be higher and the portion of shallow water from 1960 and modern shallow water is correspondingly lower.

The influence of borehole activities is seen in the tritium data which record significant tritium down to 1000 m, and even to 1420 m in samples collected by the SKB-packer sampling method. Recharge tritium values are around 22 TU such that mixing and dilution can account for the present distribution of values. However, at one level (1420 m) the presence of 26 TU (i.e. in excess of present-day recharge at 22 TU) suggests that one of the mixing end-members may be "old" tritium waters (up to 35 yrs). Mixing modelling showed that water from 1960 is the main source for tritium. The high tritium values in the 1090-1096.2 m section are due to contamination of 1% shallow water from 1960 and 2% of modern shallow water. This water may have been drawn into the borehole at various levels but mostly from above 700-1000 m depth during the hydraulic testing and the long-term maintenance pumping. Alternative explanations such as in-situ production of tritium have been considered, but this has been judged unlikely because of an absence of uranium mineralisation in the area. This phenomenon will anyhow be further investigated.

The working hypothesis at the moment is that the upper 800 m of bedrock at Laxemar lies within a groundwater recharge area; the sub-vertical to moderate angled fracture zones facilitate groundwater circulation to considerable depths, at least to 800 m, thus accounting for some of the low saline brackish groundwaters in these conducting fracture zones. Below 1100 m the system is hydraulically and geochemically "closed" such that highly saline groundwaters exist in a near-stagnant environment. These Ca-Cl dominated brines represent deep regional groundwaters where long residence times and water-rock interactions have played a dominant role in determining their composition.

1. Introduction and aims

On October 6, 1992, borehole KLX02 was drilled at Laxemar, located close to the Äspö Hard Rock Laboratory (HRL), adjacent to the Baltic coast approximately 350 km south of Stockholm (Figure 1-1). KLX02 is drilled to a depth of 1705 m, some 2.5 km WSW of Äspö and 0.62 km SW of borehole KLX01 at 1078.0 m. KLX02 represents the deepest borehole drilled within the Research and Development programme managed by the Swedish Nuclear Fuel and Waste Management Company (SKB).

Äspö is being investigated because it geologically represents a variety of typical crystalline bedrock environments in Sweden designated as suitable host rocks for the final disposal of radioactive waste. It was also selected because a laboratory should be placed close to one of the nuclear power plants where existing services and infrastructure required for research already existed. Many boreholes have been used to evaluate the geological, hydrogeological and hydrogeochemical character of the Äspö area; the deepest boreholes drilled were to depths of 1000 m.

The main aims behind locating such a deep borehole at Laxemar are:

- To increase the knowledge of rock composition, rock characteristics, groundwater flow paths and groundwater compositions at greater depths and in a wider regional context than has been possible within the Äspö project.
- To test new drilling and characterisation methods of deep >1500 m boreholes.
- To develop documentation and working procedures to be used for future site-specific characterisation programmes.

In the context of hydrochemistry the objectives are:

- To test new methods and equipment to sample deep groundwaters.
- To establish the composition and origin of deep basement groundwaters at Laxemar.
- To use these data to support existing hydraulic and hydrogeochemical interpretation of the Äspö site.
- To provide a sound basis to evaluate deep regional groundwater systems in this part of Sweden.

There was a tight schedule to carry out this programme which required thorough preparation and detailed planning. The objectives of this report are to itemise the planning procedure, to describe the borehole testing and groundwater sampling protocols, to briefly present the geological and hydrological data of the borehole, and to use these data as a basis to interpret the results of the sampled groundwater chemistry. A preliminary geochemical modelling is performed which includes; regional comparison with Äspö data, mixing modelling and mass balance calculations. Finally, the successes/failures of the sampling campaign are discussed in the light of future application to site-specific characterisation programmes.

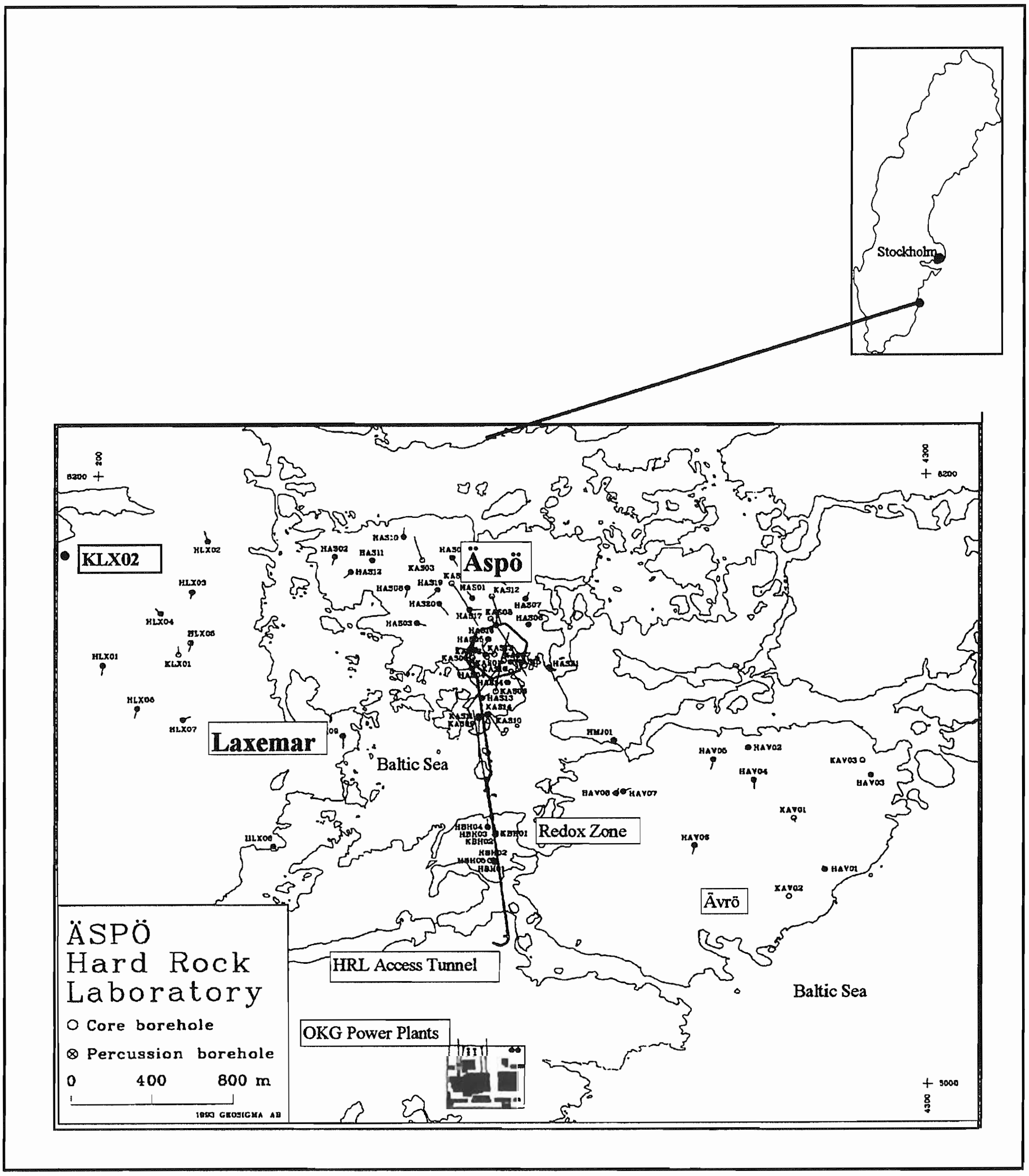


Figure 1-1: Location of Laxemar in relation to the Äspö Hard Rock Laboratory (HRL), and the position of borehole KLX02.

2. Background geological and hydrogeological information

2.1 Geology

The Laxemar region is characterised by a slightly undulating topography (~20 m.a.s.l) of well exposed rock. Borehole KLX02 is situated about 1500 m from the Baltic Sea 18.31 m.a.s.l., and borehole KLX01 is situated about 100 m from the Baltic Sea 16.81 m.a.s.l. The geology is characterised by a red to grey porphyritic granite-granodiorite of Småland type containing microcline megacrysts up to 1 to 3 cm in size. This variety belongs to the vast Transscandinavian Granite Porphyry Belt (Gåal and Gorbatschev, 1987) with intrusion ages (U, Pb) between 1760-1840 Ma (Johansson, 1988), i.e., late to post-orogenic in relation to the Svecofennian origin (1800-1850 Ma).

In common with Äspö the dominant rock-types comprise, in decreasing order of importance, Småland Granite, Äspö Diorite, Greenstone and Fine-grained Granite. In general terms, the main distinction is the virtual absence of the fine-grained granite variety at Laxemar (<1%) compared to Äspö (12-15%); in fact there is a continuous decrease of this rock-type west from Äspö to borehole KLX01 and finally to KLX02. This decrease appears to be compensated by an increase in greenstone. At Laxemar the Småland Granite type (with only minor Äspö Diorite) dominates with increasing depth to 1500 m; at Äspö the diorite increases with depth (R. Stansfors, per. comm., 1994). KLX02 is dominated by Småland Granite and Äspö Diorite, in the central parts of the borehole (600-1300 m depth) lenses of greenstone and Fine Grained Granite (Applite) occur (Figure 2-1).

Fracture frequency in borehole KLX02 is generally low down to 700-750 m and from 1100-1500 m, otherwise higher frequency can be observed; there is a strong association of fractures with crushed greenstone horizons (Figure 2-1). Generally, Laxemar is less fractured than Äspö, with KLX02 less fractured than KLX01.

Radar measurements (Carlsten, 1994) point to strong reflections at 265-270 m, 335-340 m, 384-388 m, 466-468 m, 604-609 m and 655-670 m; the underlined borehole sections correspond to hydraulically conductive zones as indicated by flow-meter measurements (Figure 2-1).

The main fracture filling mineral phases consist of, in decreasing order of frequency: group A (calcite, chlorite), group B (hematite, Fe-oxyhydroxides, epidote, fluorite), and group C (pyrite, magnetite, laumontite/prehnite, gypsum). The underlined fracture minerals are the main types found in the water conducting fractures (Figure 2-1).

2.2 Hydrogeology

The areal distribution of hydraulic conductivity at Laxemar on the site-specific scale is believed to be heterogeneous, with a significant downward gradient through a series of sub-vertical fractures, perhaps extending down to 500-700 m. This suggests that KLX02 lies within an area of active recharge, and recorded snow-melt waters down to 200-300 m in borehole KLX01 (Follin, 1993), located close to KLX02 (Figure 1-1), would support this. In contrast, the lower part of KLX02, say from 700-1700 m, is believed to represent more stagnant groundwater conditions.

Downhole hydraulic tests (5 capacity tests) were carried out between November 1992 and June 1993 (Follin, 1993). These showed that about 60% of the total discharge is recovered from the upper 250 m of bedrock and about 20% from depths below 500 m. Overall, both the specific storage coefficient and specific transmissivity decrease with depth, and that during pumping the specific storage coefficient is twice that during recovery.

Downhole groundwater logging of KLX02 (Figure 2-1) incorporated flow meter measurements to evaluate the hydraulic conductivity; these were combined with electrical conductivity and temperature observations. The logs indicate an area of very low hydraulic conductivity associated with very high salinity (1100-1650 m), an area of higher hydraulic conductivity and low electrical conductivity (surface to 800 m), and an intermediate area where there is a transition from low to high electrical conductivity (800-1100 m).

In general, all these data essentially confirm that the uppermost parts of the bedrock are clearly affected by infiltration (and hence brackish in composition) whereas the deeper parts are, in comparison, near stagnant and highly saline.

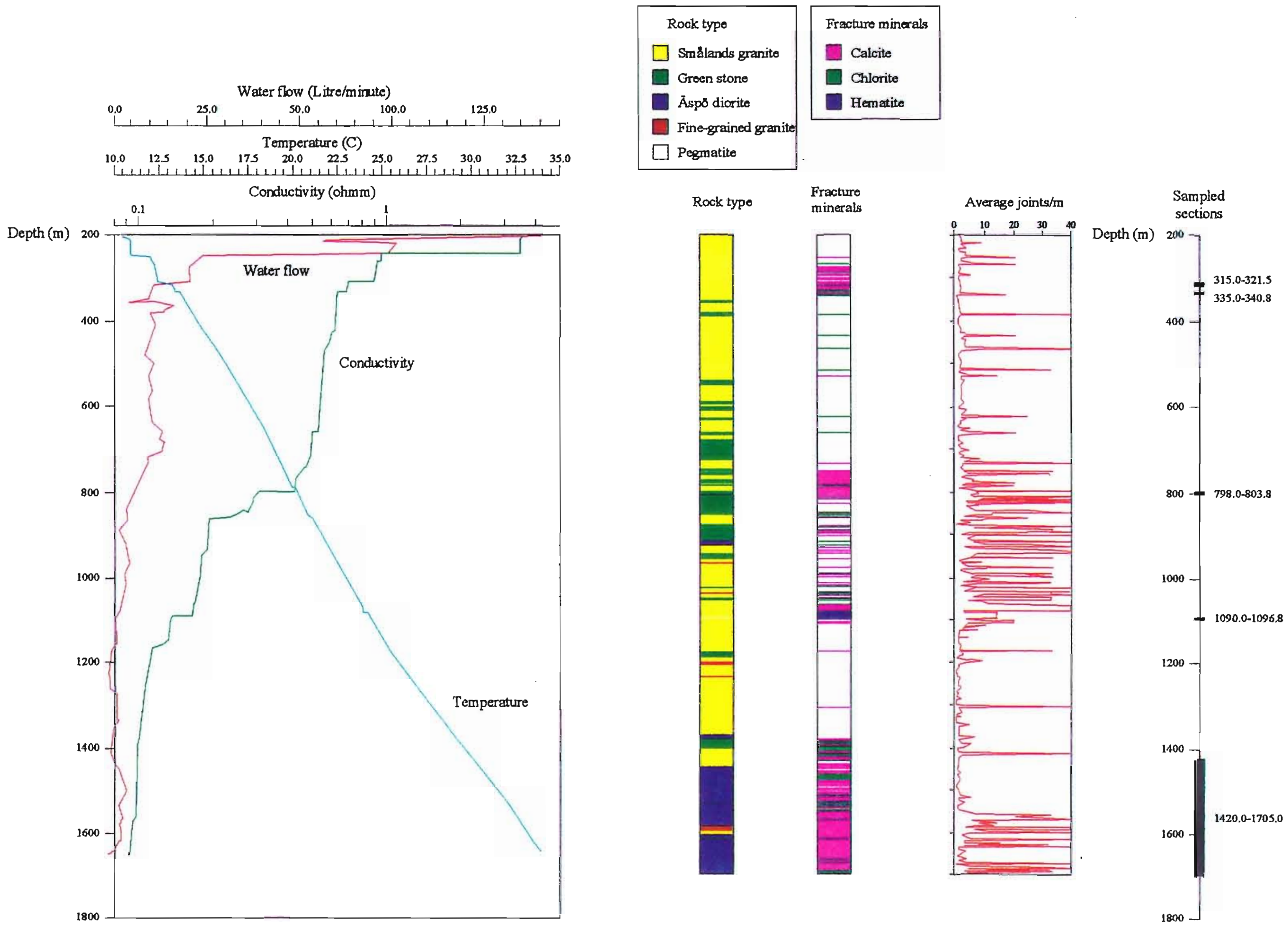


Figure 2-1: *KLX02 downhole groundwater logging profiles (water flow, temperature, electrical conductivity), core mapping (rock type, fracture minerals and average fracture frequency) and the selected borehole sections where SKB-packer sampling was conducted. The borehole section 9-1681 m were sampled with Tube sampler. The depth scale is common for all the plots.*

3. Groundwater geochemistry

3.1 Borehole activities

Figure 3-1 outlines the chronological sequence of borehole activities carried out in borehole KLX02 prior to, during and subsequent to the chemical investigation campaign performed with two different sampling methods (Tube sampler and SKB-packer sampler). This allows some estimation of possible and probable causes of contamination in the sampled groundwaters which is important when the geochemical datasets are being evaluated. Figure 3-1 shows that drilling and borehole cleaning by air-lift pumping were completed by December of 1992. Maintenance pumping (pump set at 100 m in casing) was conducted periodically over a period of 181 days between December 1992 and June 1993 at an extraction rate of 2.95 L/sec. During July 1993 downhole activities included radar measurements and geophysical logging, both of which are known to perturb the borehole groundwater environment. These activities were immediately followed by open-hole hydrochemical sampling using the tube sampling method in August 1993, followed by downhole TV characterisation of the borehole. Complete hydrochemical sampling from isolated borehole sections was conducted with the SKB-packer sampler four months later in November 1993.

At least four potential sources of contamination by mixing may be reflected in the groundwaters sampled for hydrochemical characterisation: a) during drilling and the maintenance pumping carried out during and after drilling, b) open-hole effects during borehole inactivity following drilling, in particular the influence of brackish water entering the borehole at the hydraulically active 220 m level and density differences due to strongly increasing salinity with depth, c) the influence of the maintenance pumping and pumping during the flow meter measurements, and d) perturbation of the open-hole groundwater during downhole geophysical logging. The possible effects of these processes on the representativeness of the groundwater samples are discussed below (section 3.4).

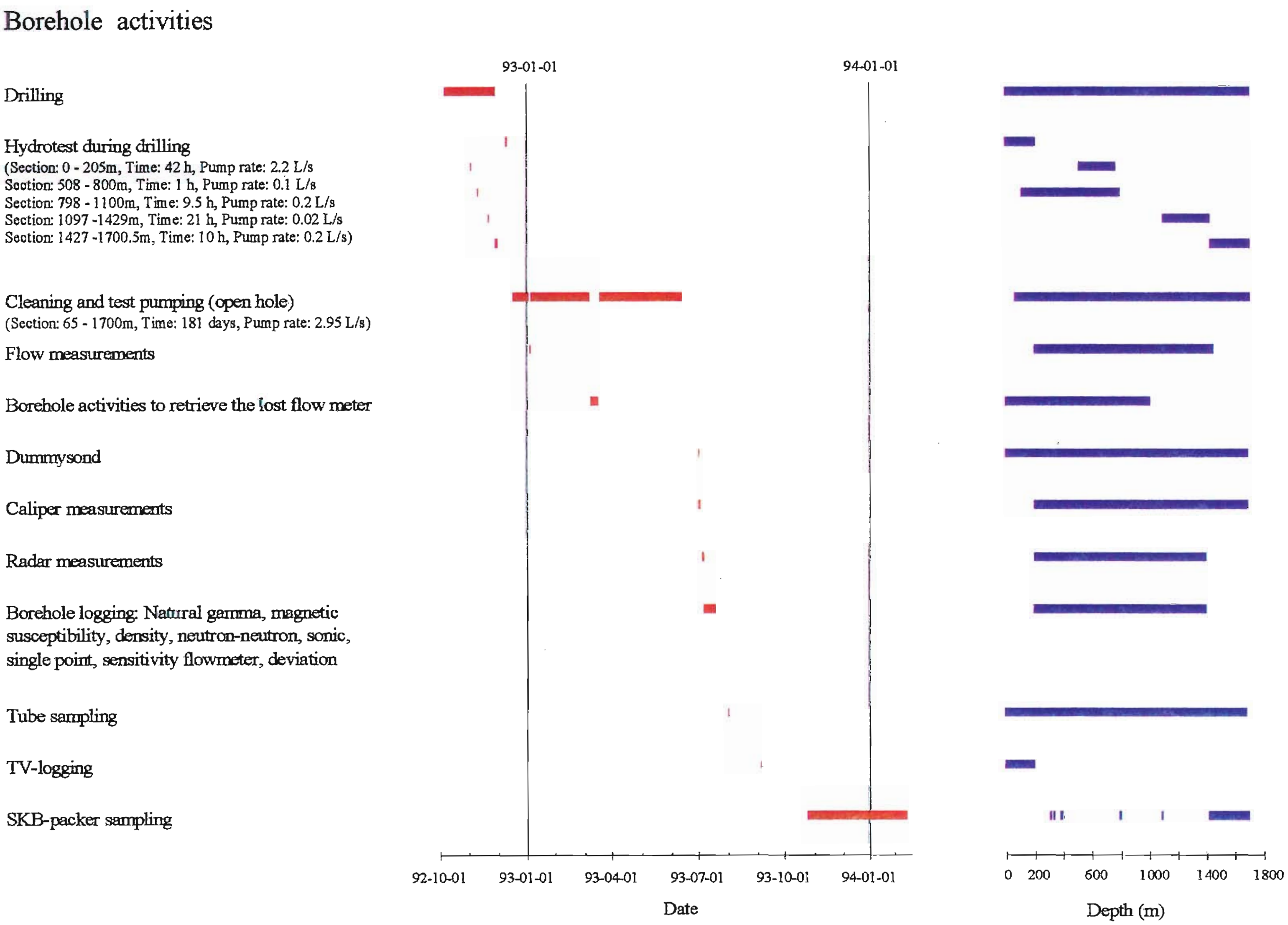


Figure 3-1: Chronological sequence of activities carried out in borehole KLX02

3.2 Groundwater sampling methods

Groundwater sampling was conducted on two occasions and using different methods. The first sampling was taken in August 3rd, 1993 by Müllern et al. (pers. comm. 1993) in the open borehole using the so-called Tube sampler (Nurmi and Kukkonen, 1986). This consists of 50 m sections of polyamide tubes (10 mm outer diameter; maximum length 1700 m) with a hand operated valve and connector fastened at the both ends of each tube. The first string placed in the borehole contains a check-valve; the following tube is connected to the upper part of the tube in the borehole and the hand operated valves are open. Several tube strings are connected until the desired measuring depth is achieved (i.e. to 1681 m in KLX02) (Figure 3-2). It is important to note that only the water column in the open borehole is sampled; no pumping is involved. When the tube string is filled with borehole water the individual lengths are isolated by closing the valves and subsequently removed; water contained in the 50 m tube lengths (1 litre) is poured into flasks for analysis.

The advantage of this technique is that the equipment is convenient, easy and rapid to operate, even down to considerable depths. The disadvantage is that the water column collected represents open-hole conditions, i.e. the chemical distribution in the groundwater is controlled by the hydraulic properties of the borehole, which may not always conform to adjacent bedrock conditions. Furthermore, lowering the tube into the open borehole may cause perturbation and mixing of groundwater types around and inside the tube. In the following text, tables and figures **Tube sampler** is used when referring to activities or samples taken with this equipment.

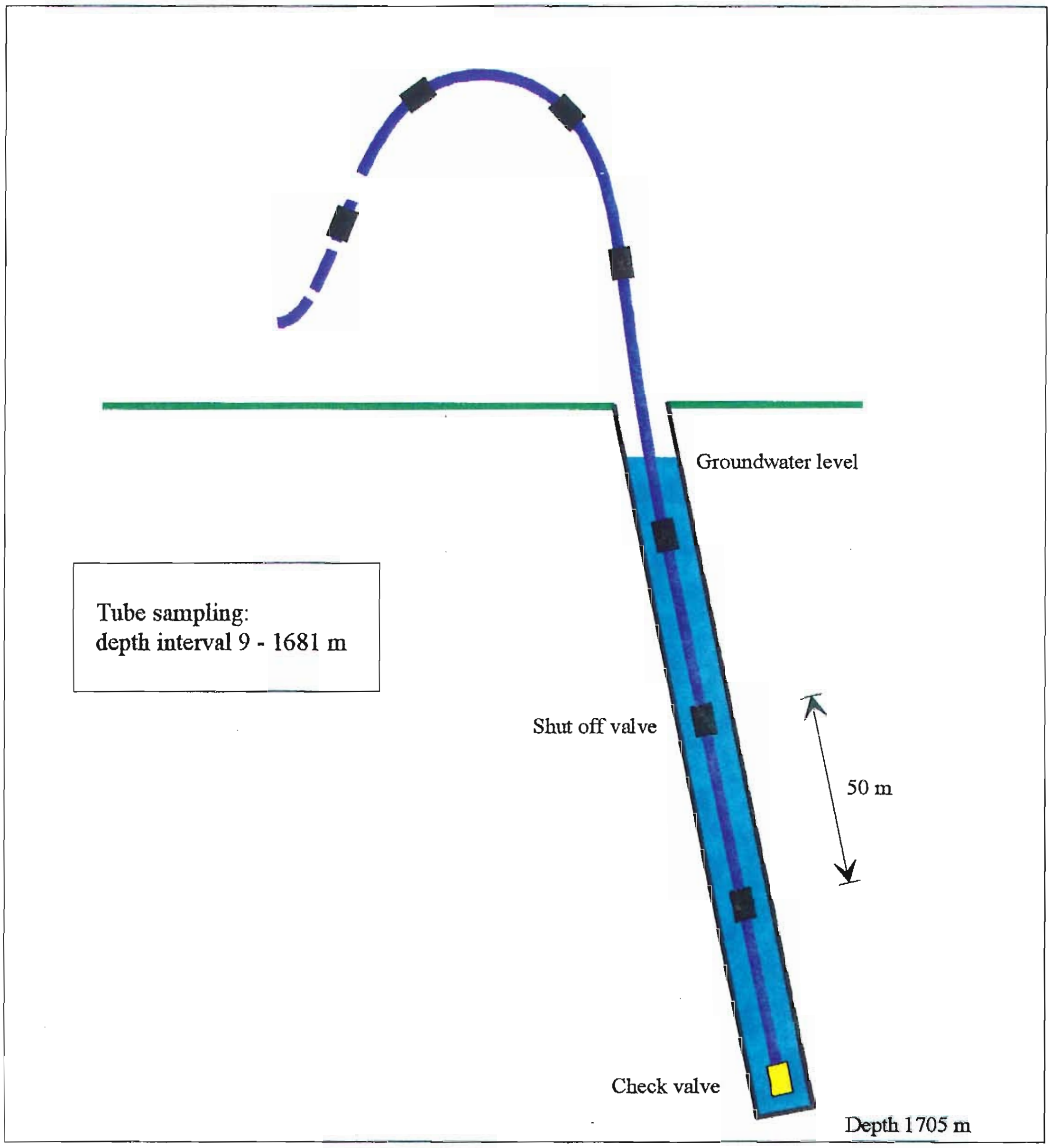


Figure 3-2: *Diagrammatic representation of the Tube sampler.*

The second sampling, from the first of November 1993 to the fifth of January 1994, was carried out using the SKB Mobile Field Laboratory. The Mobile Field Laboratory includes a chemical laboratory unit, hose unit/units, borehole equipment, packer units and the CHEMMAC measuring system. The borehole equipment was modified for greater depths (Figure 3-3). The basic Mobile Field Laboratory equipment is essentially similar to that described by Almén et al. (1986) Axelsen et al. (1986) and Wikberg (1987). Updated documentation is given in "Manual för Mobilt Fältlaboratorium" belonging to a series of SKB manuals and method descriptions (SKB MD 430-434). In the following text, tables and figures **SKB-packer sampler/equipment** is used when referring to activities or samples conducted with the mobile field laboratory.

During the second sampling campaign the groundwater was pumped up from chosen water-conducting sections in the bedrock sealed off by inflatable rubber packers with an adjustable straddle length. The hydraulic conductivity of these sections averaged between 10^{-8} ms^{-1} and 10^{-6} ms^{-1}. A hydraulically operated piston pump, which gives a maximum flow of about 250 mL/min from the isolated borehole section, has the capacity of reducing the pressure within the sampled section by more than 10 bar (100 mwc). The Eh and pH values were monitored both at the bedrock surface, where the water is pumped through a flow-through cell (surface CHEMMAC) located in the mobile laboratory, and by a downhole probe CHEMMAC (Eh and pH) located within the sampling interval of the packer unit. Three different types of Eh probe were used: gold, platinum and glassy carbon. To accommodate the Laxemar borehole this set-up was modified according to Figure 3-3.

Following installation of the packers and the downhole equipment the pump is started and the capacity adjusted to give as high a water flow as possible without exceeding a pressure drawdown of 5 bar (50 mwc). At Laxemar a 1 bar (10 mwc) of under-pressure was generally used. Pumping is continued until the "dead" water volume between the packer and tubes is removed and a stable groundwater composition is achieved, on average after at least two days. Stable conditions are often determined by unchanging electrical conductivity of the groundwater. When stability is achieved, it is often the continuous change in composition of the main constituents that determine the length of the ensuing sampling and pumping period. At Laxemar, because of the tight time schedule, a full monitoring programme was not possible at every sampled section. In general, 1-2 weeks were allocated to each section at flow-rates which varied between 117-172 mL/min; in most cases this proved to be adequate.

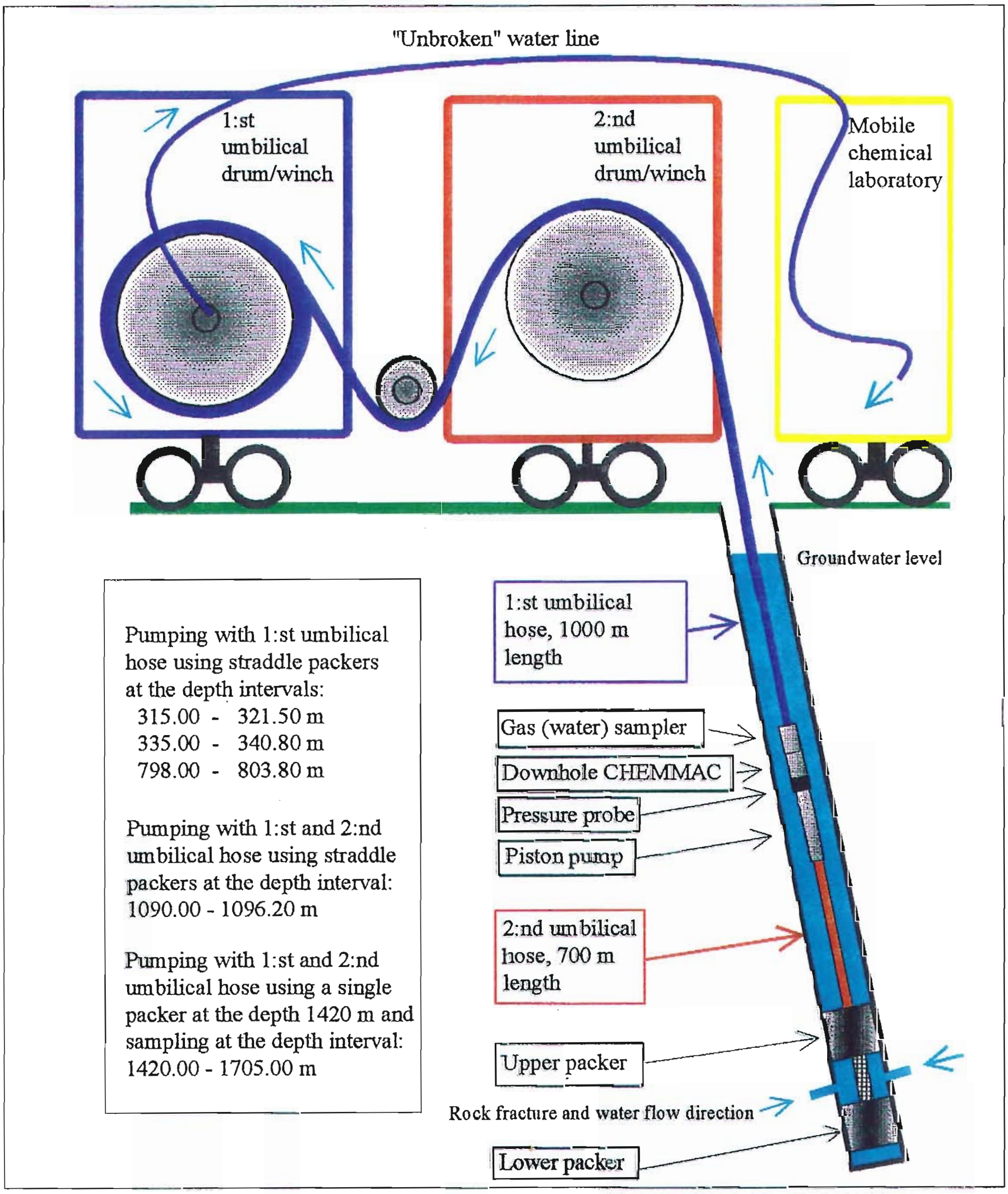


Figure 3-3: *The SKB-packer sampler equipment within the SKB Mobile Field Laboratory unit modified for sampling at greater depths. The downhole CHEMMAC probe houses the Eh and pH electrodes.*

Selection of borehole sections for groundwater sampling was based primarily on geological evidence (e.g. detailed drillcore mapping) supported by flow meter measurements and recorded downhole logging of electrical conductivity and temperature (Figure 2-1). Of the selected sections most were associated with crushed greenstone horizons or at the contact between greenstone and granite. The five selected borehole sections and the period of borehole activities during sampling are shown in Figure 3-4. The sampling programme is outlined in Table 3-1 and the timetable in Table 3-2.

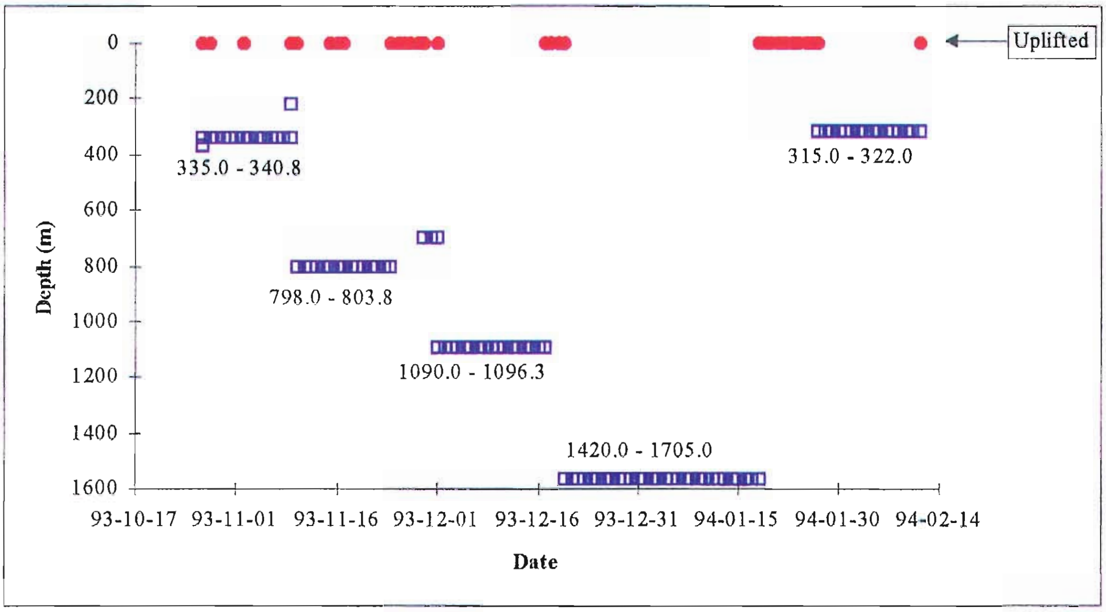


Figure 3-4: The five selected borehole sections and the period of borehole activities during sampling using the SKB-packer sampler. The selected borehole sections were based on available chemical, hydrological and geological information shown in Figure 2-1.

Table 3-1: Groundwater sampling programme carried out in KLX02 using the SKB-packer sampler.

Ground-water sampling activity no.	**Drilling water conc.**	**IonChrom. Titration: Cl, HCO_3, Br, SO_4**	**Photometry: Fe, HS- (NO_2- PO_4)**	**ICP Cataions**	**Trace elements**	**Isotopes: Uran Th, C-13, O-18, D, Tr, Sr, S**	**Spec Isotopes: 3He, 4He, Tr**	**Colloids**	**Organic Matter, Gas**	**Gas, Gas Isotopes and Bacteria**
1									o	
2	x	x	x	x						
3	x	x								
4					o					
5							o			
6						x				
7								x		
8								o		
9										o

(x = all sampling sections; O = some sampling sections)

Table 3-2: Time schedule, borehole and groundwater sampling activity. The groundwater sampling activity numbers used are taken from Table 3-1.

Date	**Section (m)**	**Groundwater sampling activity no/ borehole activities**	**Date**	**Section (m)**	**Groundwater sampling activity no/ borehole activities**
October, 27	388 - 393	lowering; pumping - no water; unstable packer pressure; uplifting to 335 m; pumping	***December***		
October, 28	335.0 - 340.8	uplifting; packer repair; lowering; pumping; starting CHEMMAC measurement	1 We	1090.0 - 1096.2	lowering; packer inflation; low packer pressure; uplifting; maintenance; lowering; pumping
			2 Th	1090.0 - 1096.2	starting CHEMMAC measurement; 2
November			3 Fr	1090.0 - 1096.2	3
1 Mo	335.0 - 340.8	3	**4 Sa**	1090.0 - 1096.2	
2 Tu	335.0 - 340.8	uplifting; pump repair; lowering; pumping	**5 Su**	1090.0 - 1096.2	
3 We	335.0 - 340.8	2	6 Mo	1090.0 - 1096.2	no packer pressure; gas leakage; packer inflation
4 Th	335.0 - 340.8	3	7 Tu	1090.0 - 1096.2	2
5 Fr	335.0 - 340.8	2	8 We	1090.0 - 1096.2	3; 8
6 Sa	335.0 - 340.8		9 Th	1090.0 - 1096.2	1; 2; 8
7 Su	335.0 - 340.8		10 Fr	1090.0 - 1096.2	1
8 Mo	335.0 - 340.8	2; 4; 6	**11 Sa**	1090.0 - 1096.2	1
9 Tu	335.0 - 340.8	3; 7; stopping CHEMMAC measurement; uplifting; packer repair; lowering to 220 m	**12 Su**	1090.0 - 1096.2	1
10 We	798.0 - 803.8	lowering; pumping; starting CHEMMAC measurement	13 Mo	1090.0 - 1096.2	1; low packer pressure; gas leakage; packer inflation; 3; unrepresentative sampling
11 Th	798.0 - 803.8	2	14 Tu	1090.0 - 1096.2	1; 2; 4
12 Fr	798.0 - 803.8	1; 3	15 We	1090.0 - 1096.2	1; 3
13 Sa	798.0 - 803.8	1	16 Th	1090.0 - 1096.2	1; 2; 4; 6
14 Su	798.0 - 803.8	1	17 Fr	1090.0 - 1096.2	1; 7; 9; stopping CHEMMAC measurement; uplifting; gas sampler/pump repair
15 Mo	798.0 - 803.8	1; 2; uplifting; packer repair; lowering; pumping	**18 Sa**		
16 Tu	798.0 - 803.8	low packer pressure; packer deflation; uplifting; packer repair; lowering; pumping	**19 Su**		
17 We	798.0 - 803.8	no water flow; uplifting; check valve repair; lowering; pumping	20 Mo	1420.0 - 1705.0	lowering; pumping; starting CHEMMAC measurement
18 Th	798.0 - 803.8	1; 2	21 Tu	1420.0 - 1705.0	
19 Fr	798.0 - 803.8	1; 3	22 We	1420.0 - 1705.0	2
20 Sa	798.0 - 803.8	1	23 Th	1420.0 - 1705.0	
21 Su	798.0 - 803.8	1	24 Fr	1420.0 - 1705.0	
22 Mo	798.0 - 803.8	1	**25 Sa**	1420.0 - 1705.0	
23 Tu	798.0 - 803.8	1; 2; 4; 6	**26 Su**	1420.0 - 1705.0	
24 We	798.0 - 803.8	3; 7; 9; stopping CHEMMAC measurement; uplifting	27 Mo	1420.0 - 1705.0	
25 Th		gas sampler/pump repair; establishing of equipment	28 Tu	1420.0 - 1705.0	1; 2
26 Fr		establishing of equipment	29 We	1420.0 - 1705.0	1
27 Sa			30 Th	1420.0 - 1705.0	1
28 Su		establishing of equipment	31 Fr	1420.0 - 1705.0	1
29 Mo	~700	lowering; packer inflation			
30 Tu	~700	establishing of equipment			

Table 3-2: Continued Time schedule, borehole and groundwater sampling activity. The groundwater sampling activity numbers used are taken from Table 3-1.

Date	Section (m)	Groundwater sampling activity no/ borehole activities	Date	Section (m)	Groundwater sampling activity no/ borehole activities
January			*February*		
1 Sa	1420.0 - 1705.0	1	1 Tu	315.0 - 322.0	1; 2
2 Su	1420.0 - 1705.0	1	2 We	315.0 - 322.0	1
3 Mo	1420.0 - 1705.0	1	3 Th	315.0 - 322.0	1
4 Tu	1420.0 - 1705.0	1; 2	4 Fr	315.0 - 322.0	1
5 We	1420.0 - 1705.0	1; 3	**5 Sa**	315.0 - 322.0	1
6 Th	1420.0 - 1705.0	1	**6 Su**	315.0 - 322.0	1
7 Fr	1420.0 - 1705.0	1	7 Mo	315.0 - 322.0	1
8 Sa	1420.0 - 1705.0	1	8 Tu	315.0 - 322.0	1; 2
9 Su	1420.0 - 1705.0	1	9 We	315.0 - 322.0	1; 3; 8; 9
10 Mo	1420.0 - 1705.0	1	10 Th	315.0 - 322.0	2; 4; 6; 8
11 Tu	1420.0 - 1705.0	1; 3	11 Fr	315.0 - 322.0	5; 9; stopping CHEMMAC measurement; uplifting
12 We	1420.0 - 1705.0	1; 3			
13 Th	1420.0 - 1705.0	1; 3; 7; 8			
14 Fr	1420.0 - 1705.0	2; 8			
15 Sa	1420.0 - 1705.0				
16 Su	1420.0 - 1705.0				
17 Mo	1420.0 - 1705.0	2; 5; 4; 6			
18 Tu	1420.0 - 1705.0	2; 4; 9; stopping CHEMMAC measurement; uplifting			
19 We		establishing of equipment			
20 Th		establishing of equipment			
21 Fr		establishing of equipment			
22 Sa		establishing of equipment			
23 Su		establishing of equipment			
24 Mo		establishing of equipment			
25 Tu		establishing of equipment			
26 We		packer repair			
27 Th	315.0 - 322.0	lowering; pumping; starting CHEMMAC measurement			
28 Fr	315.0 - 322.0	packer leakage; deflate and inflate of packer; 1			
29 Sa	315.0 - 322.0	1			
30 Su	315.0 - 322.0	1			
31 Mo	315.0 - 322.0	1; 2			

3.3 Groundwater analysis

3.3.1 Results and procedures

3.3.1.1 Tube sampler results

The samples from the tube sampling were analysed for major components by using ICP-AES and standard titration methods; tritium, deuterium and oxygen-18 were also determined. No in situ filtration or preservation was performed; this was carried out before the ICP analyses. There was a delay of three or four days in measuring alkalinity and pH which has affected the accuracy of the pH values due to uptake or loss of CO_2. The results of the tube sample analyses are given in Table 3-3; in Appendix 1 the results are shown as matrix scatter plots with histograms. This is an excellent way to see at a glance the general trends of the analytical data.

Table 3-3: Chemical analyses of samples collected using the Tube sampler (mg/L).

IDCODE	SECUP	SECLOW	DATE	Na	K	Ca	Mg	HCO_3	Cl	SO_4-S	Si	Sr	Li	pH^*	δ^2H smow	$^3H^{**}$ TU	$^3H^{***}$ TU	$\delta^{18}O$ smow
KLX02	9	31	930803	137	3.9	54.1	4.37	220	149	20.4	3.5	0.61	0.020	**6.6**	-74.4	8.4		-9.90
KLX02	31	81	930803	134	3.9	45.7	4.34	202	146	19.4	4.0	0.58	0.019	**6.6**	-75.1	5.9		-10.50
KLX02	81	131	930803	130	3.8	43.4	4.33	200	140	18.9	4.3	0.57	0.019	**6.9**	-74.6	4.2		-10.70
KLX02	131	181	930803	120	3.7	39.3	4.33	200	123	17.5	4.5	0.51	0.017	**7.0**	-76.3	12		-10.30
KLX02	181	231	930803	110	4.3	38.6	4.31	202	109	16.3	5.1	0.50	0.016	**6.9**	-76.1	15		-10.40
KLX02	231	281	930803	97.4	3.5	33.8	4.30	202	82.5	14.6	5.5	0.41	0.014	**7.2**	-76.3	13		-10.50
KLX02	281	331	930803	87.0	3.5	31.5	4.30	205	63.8	13.4	5.7	0.36	0.012	**7.2**	-75.9	5.1		-10.50
KLX02	331	381	930803	77.0	3.5	29.1	4.35	205	45.0	12.2	6.3	0.30	0.010	**7.2**	-75.4	7.6		-10.70
KLX02	381	431	930803	72.9	3.4	27.4	4.54	205	34.5	11.2	6.4	0.26	0.009	**7.2**	-76.4	7.6		-10.70
KLX02	431	481	930803	69.5	3.4	26.2	4.62	204	28.0	10.7	6.5	0.23	0.009	**7.2**	-75.5	8.4		-10.60
KLX02	481	531	930803	67.7	3.5	25.6	4.66	202	26.5	10.4	6.9	0.21	0.009	**7.2**	-76.2	13		-10.60
KLX02	531	581	930803	67.3	3.5	25.3	4.65	198	26.2	10.2	6.9	0.20	0.008	**7.3**	-75.3	16		-10.60
KLX02	581	631	930803	67.6	3.4	25.5	4.53	201	25.5	9.94	6.8	0.20	0.008	**7.3**	-76.5	8.4		-10.40
KLX02	631	681	930803	67.4	3.4	25.3	4.55	200	28.0	9.93	6.8	0.20	0.008	**7.3**	-75.5	8.4		-10.40
KLX02	681	731	930803	68.2	3.5	25.5	4.55	200	28.3	9.96	7.1	0.20	0.008	**6.4**	-76.0	18		-10.40
KLX02	731	781	930803	67.6	3.4	25.9	4.55	209	28.0	10.0	6.8	0.21	0.007	**6.8**	-76.6	19		-10.50
KLX02	781	831	930803	68.8	3.4	28.3	4.50	202	34.0	10.4	6.8	0.26	0.009	**6.9**	-75.5	15		-10.50
KLX02	831	881	930803	73.4	3.4	38.9	4.34	205	60.0	11.8	6.8	0.46	0.013	**7.0**	-75.1	13		-10.70
KLX02	881	931	930803	103	3.4	82.6	4.47	202	175	16.1	6.5	1.22	0.025	**7.0**	-76.1	11		-10.40
KLX02	931	981	930803	327	3.7	397	4.61	181	1080	41.9	6.2	6.90	0.119	**6.9**	-77.8	14		-10.70
KLX02	981	1031	930803	1000	5.1	1340	4.68	126	3780	101	5.6	23.4	0.380	**6.8**	-81.5	11		-11.30
KLX02	1031	1081	930803	2460	8.5	3590	3.95	52.8	9910	215	4.4	59.0	0.938	**6.6**	-84.5	10		-11.90
KLX02	1081	1131	930803	3300	11.3	4820	3.16	23.8	13600	269	4.0	83.0	1.41	**6.7**	-85.2	<4.2		-12.10
KLX02	1131	1181	930803	3780	10.5	5720	2.48	13.4	16000	300	3.7	100	1.56	**6.7**	-83.7	5.1	0.23	-12.00
KLX02	1181	1231	930803	3930	10.2	6110	2.22	12.2	16800	310	3.7	101	1.49	**6.4**	-82.3	<4.2		-12.00
KLX02	1231	1281	930803	4190	12.0	6810	2.11	10.9	18500	317	3.6	118	1.83	**6.6**	-80.7	<4.2	<0.2	-11.90
KLX02	1281	1331	930803	4640	14.2	8000	2.61	10.6	21500	315	4.0	141	2.26	**6.7**	-77.1	<4.2		-11.40
KLX02	1331	1381	930803	5750	18.2	11000	2.16	10.2	29100	317	4.1	205	2.83	**6.7**	-66.0	<4.2	<0.2	-10.40
KLX02	1381	1431	930803	6520	20.5	12700	2.28	10.8	33100	319	4.2	220	2.94	**6.9**	-60.2	<4.2		-9.90
KLX02	1431	1481	930803	7330	25.6	15800	2.62	11.5	39700	316	3.8	281	3.92	**7.0**	-53.2	<4.2	<0.2	-9.50
KLX02	1481	1531	930803	7740	30.6	17100	3.07	11.6	43300	309	3.7	313	4.18	**7.1**	-49.4	<4.2		-9.80
KLX02	1531	1581	930803	7690	30.0	16900	2.88	11.2	43500	305	3.9	311	4.20	**7.2**	-49.8	<4.2	<0.2	-9.00
KLX02	1581	1631	930803	7860	34.2	17500	2.85	10.5	44800	305	3.8	316	4.20	**7.3**	-48.1	<4.2		-9.10
KLX02	1631	1681	930803	8200	45.5	19200	2.12	14.1	47200	302	2.9	337	4.64	**7.3**	-44.9	<4.2	<0.2	-8.90

Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section, DATE = Sampling date, SO_4-S = Sulphur by ICP-AES, pH = Field measurement. * = The reported pH values are in **bold** print indicating risk of error. ** = The reported values are recalculated from Bq/L using the relation 1 Bq = 8.45 TU, analysed by Energiteknikk, Kjeller; for detection limit see Table 3-6. *** = Tritium analysed by GSF-Institut, Neuherberg; for detection limit see Table 3-6.

3.3.1.2 SKB-packer sampler results

Analyses of the water samples collected are given in Table 3-4; in Appendix 2 the results are shown as matrix scatter plots with histograms.

Using the SKB-packer sampler, the groundwater was constantly pumped up to the laboratory unit and samples for immediate analysis in the field as well as samples for external laboratory analysis were taken according to Table 3-4. All water collected during one day was labelled with the same sample number. The groundwater passed through an on-line 0.45 μm filter before it was collected for analyses. However, when water for iron and ICP analysis was collected, a 0.45 μm single-use polycarbonate filter was used.

Some of the major components (the anions), pH and electrical conductivity were determined daily in the field laboratory to achieve an immediate feed-back of the groundwater composition. This allows the analytical protocol to be modified if required. Ferrous and ferric iron and minor anions were also determined in the field laboratory but not as frequent. The system enables the redox sensitive components to be determined immediately without atmospheric contamination. Water for iron determination in the field and for ICP-AES analyses was collected in one acidified (1% supra pure HCl), acid washed bottle and then divided into different portions. Extra precautions were taken to avoid contamination of the acidified samples collected for trace element analysis by ICP-MS. Sample bottles (Winkler) for sulphide determination were preserved using sodium hydroxide and zinc acetate.

The analytical methods, laboratories and detection limits used when sampling with the SKB-packer sampler are listed in Table 3-5 and Table 3-6. Several components were determined by more than one method for quality control.

Table 3-4: Chemical analyses of samples collected using the SKB-packer sampler (mg/L). The grey marked fields indicate the most representative samples.

IDCODE	SECUP (m)	SECLOW (m)	SNO	DATE	Na	K	Ca	Mg	HCO_3	Cl	F	SO_4	SO_4-S	Br	Si	Fe	Fe(tot)	Fe(+II)	Mn	Li	Sr	pH
KLX02	315.00	321.50	2734	940131	74	3.1	25	4.6	218	33	2.6	29	9	0.13	7.1	1.88	1.900	1.880	0.20	0.03	0.24	7.7
KLX02	315.00	321.50	2735	940201	78	3.1	25	4.7	220	38		23	10	0.16	7.1	1.77	1.770	1.740	0.19	0.01	0.21	7.7
KLX02	315.00	321.50	2736	940208	106	3.2	25	4.6	223	69	3.6	46	17	0.35	6.9	1.16	1.150	1.140	0.16	0.01	0.23	7.8
KLX02	315.00	321.50	2737	940209					223	71	4.0	44		0.28			1.110	1.110				7.8
KLX02	315.00	321.50	2738	940210	111	3.1	24	4.6	223	73		43	20	0.23	7.0	1.06	1.050	1.040	0.15	0.01	0.23	7.8
KLX02	335.00	340.80	2701	931101	130	12.3	32	5.9	211	126		51	19	0.26	6.9	0.802	0.760	0.746	0.20	0.03	0.28	7.8
KLX02	335.00	340.80	2702	931103					205	159	4.0	53		0.37								7.9
KLX02	335.00	340.80	2703	931104	170	3.4	35	6.1	206	178	4.2	77	24	0.51	6.7	0.675	0.686	0.675	0.18	0.03	0.32	
KLX02	335.00	340.80	2704	931105					201	200	4.3	97		0.56								7.6
KLX02	335.00	340.80	2705	931108	206	3.1	36	5.9	201	235	4.3	84	29	0.67	6.4	0.465	0.464	0.464	0.14	0.03	0.39	8.2
KLX02	335.00	340.80	2706	931109					201	245		92		0.82								8.0
KLX02	798.00	803.80	2707	931111	416	3.5	115	8.7	95	717		199	65	2.2	6.3	1.12	1.160	1.160	0.23	0.09	1.66	7.7
KLX02	798.00	803.80	2708	931112					94	701	4.0	183		2.3								7.6
KLX02	798.00	803.80	2709	931115	308	4.3	115	10.6	104	593	3.7		46	3.3	7.0	1.77	1.790	1.790	0.36	0.06	1.46	7.8
KLX02	798.00	803.80	2710	931118	108	2.7	31	4.6	196	87	2.9	65	15	0.5	7.0	0.585	0.566	0.540	0.19	0.01	0.32	7.7
KLX02	798.00	803.80	2711	931119					157	269	2.7	69		1.1								
KLX02	798.00	803.80	2712	931123	288	4.5	123	10.6	111	548	3.2	105	37	2.4	7.5	1.83	1.730	1.710	0.39	0.08	1.66	7.6
KLX02	798.00	803.80	2713	931124					105	577	3.8	109		2.5								7.6
KLX02	1090.00	1096.20	2714	931202	3260	10.6	4730	3.2		12300		827	289	72	4.7	0.014	0.044	0.032	0.07	1.67	81.6	7.0
KLX02	1090.00	1096.20	2715	931203						14200		968		111								8.1
KLX02	1090.00	1096.20	2716	931207	3760	10.8	5660	1.8	7.0	14600		934	317	103	5.3	0.034	0.047	0.043	0.02	2.01	95.1	8.3
KLX02	1090.00	1096.20	2717	931208					8.2	14600		866		112			0.010	0.003				8.5
KLX02	1090.00	1096.20	2718	931209	3770	10.8	5710	2.1	8.2	14500		970	320	111	5.5	0.002	0.012	0.007	0.02	1.99	96.2	8.5
KLX02	1090.00	1096.20	2719	931213						15500	1.5	698		91			0.365	0.371				7.7
KLX02	1090.00	1096.20	2720	931214	3750	10.9	5670	1.9	8.1	15600	1.5	1135	320	125	5.4	<0.002	0.007	0.003	0.02	1.94	95.6	8.4
KLX02	1090.00	1096.20	2721	931215					8.6	15500		973		110			0.007	0.002				8.4
KLX02	1090.00	1096.20	2722	931216	3800	10.4	5620	2.1	8.5	15800	1.4	1010	309	130	5.2	<0.002			0.01	2.16	97.4	8.5
KLX02	1420.00	1705.00	2723	931222	6270	30.6	12300	2.0	8.3	29100	1.2	995	332	233	4.3		0.069	0.067	0.12	5.67	340	6.4
KLX02	1420.00	1705.00	2724	931228	8170	30.5	19400	2.5		42200	1.6	683	310	325	4.3		0.028	0.027	0.12	5.63	340	7.8
KLX02	1420.00	1705.00	2725	940104	8090	30.0	19200	2.6		45400	1.6	882	310	313	4.8	0.036			0.12	5.54	331	8.0
KLX02	1420.00	1705.00	2726	940105	8070	29.6	19200	2.7		45400	1.4	676	311	246	4.8	0.047	0.084	0.084	0.12	5.53	329	7.8
KLX02	1420.00	1705.00	2727	940111	8150	30.0	18900	2.7	12.0	45300	1.3	909	312	324	4.8	0.401	0.443	0.446	0.13	5.70	340	7.8
KLX02	1420.00	1705.00	2728	940112	8010	30.0	18600	2.5		44100	1.6	946	311	315	5.1	0.461	0.544	0.536	0.11	5.39	340	7.8
KLX02	1420.00	1705.00	2729	940113	8120	29.0	18800	2.5		45400	1.6	926	312	319	4.9	0.425	0.452	0.462	0.13	5.43	341	7.9
KLX02	1420.00	1705.00	2730	940114	8000	29.0	18600	2.5		45100	1.6	816	315	308	4.8	0.529	0.566	0.572	0.13	5.30	336	7.8
KLX02	1420.00	1705.00	2731	940117	8030	29.0	18600	2.7	9.0	45500	1.6	832	317	312	4.8	0.405	0.428	0.426	0.14	5.38	340	7.9
KLX02	1420.00	1705.00	2732	940118	8010	29.0	18500	2.7		46000		808	315	301	4.8	0.325	0.346	0.348	0.13	5.38	343	7.9

Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section, SNO = Sample number, DATE = Sampling date, SO_4-S = Sulphur by ICP-AES, Fe = Total Iron by ICP-AES, Fe(tot) = Total Iron by the Ferrozine method, pH = Manual measurement of pH in the laboratory.

Table 3-4: Continued. Chemical analyses of samples collected using the SKB-packer sampler (mg/L). The grey marked fields indicates the most representative samples.

IDCODE	SECUP (m)	SECLOW (m)	SNO	DATE	PO_4P	NO_2N	NH_4N	HS^-	DOC*	Eh** (mV)	IONBAL	^{3}H*** TU	δ^{2}H smow	δ^{18}O smow	^{238}U (mBq/kg)	^{235}U (mBq/kg)	^{234}U (mBq/kg)	COND (mS/m)	WFLOW (mL/min)	DRILLW (%)
KLX02	315.00	321.50	2734	940131	<0.01	<0.001	0.13	<0.01			-2.43							49	162	0.14
KLX02	315.00	321.50	2735	940201		<0.001	0.10				0.16							51	164	
KLX02	315.00	321.50	2736	940208	0.02	<0.001	0.10	0.03	5.7±0.2		-2.95							68	155	0.22
KLX02	315.00	321.50	2737	940209				0.04										66	153	
KLX02	315.00	321.50	2738	940210	0.03	<0.001	0.10	0.04	5.5±0.2	~-100 (-339)	-0.65	5.9	-73.4	-10.3	11.7	0.63	34.6	70	155	0.22
KLX02	335.00	340.80	2701	931101							0.06								120	0.24
KLX02	335.00	340.80	2702	931103														137	137	0.20
KLX02	335.00	340.80	2703	931104				0.03			-2.33									
KLX02	335.00	340.80	2704	931105														145	142	0.22
KLX02	335.00	340.80	2705	931108				<0.01		~-40 (-387)	-2.40	13	-75.7	-10.6	7.2	0.33	22.4	156	142	0.24
KLX02	335.00	340.80	2706	931109														154	139	
KLX02	798.00	803.80	2707	931111				0.03			-2.44							225	112	0.36
KLX02	798.00	803.80	2708	931112														208	117	0.36
KLX02	798.00	803.80	2709	931115				<0.01			-3.18							170	164	
KLX02	798.00	803.80	2710	931118	<0.01	<0.001	<0.01	<0.01			-3.29							75	169	0.16
KLX02	798.00	803.80	2711	931119														113	172	
KLX02	798.00	803.80	2712	931123	<0.01	<0.001	0.07	<0.01	5.0±0.2	~-120 (-317)	0.24	8.4	-78.7	-10.9	10.7	0.42	25.3	143	156	0.18
												21	-78.3	-10.9						
KLX02	798.00	803.80	2713	931124														148	160	0.22
KLX02	1090.00	1096.20	2714	931202							2.03							3140	144	
KLX02	1090.00	1096.20	2715	931203														3180	140	0.24
KLX02	1090.00	1096.20	2716	931207	**0.05**			**<0.01**			1.81							3210	144	
KLX02	1090.00	1096.20	2717	931208	**0.06**	**<0.001**		**0.02**										3120	143	0.10
KLX02	1090.00	1096.20	2718	931209							2.36							3160	153	0.10
KLX02	1090.00	1096.20	2719	931213			**<0.01**											3080	150	0.26
KLX02	1090.00	1096.20	2720	931214	**0.813**	**<0.001**	**<0.01**	**<0.01**			-1.83							3340	149	
KLX02	1090.00	1096.20	2721	931215			**<0.01**											3320	153	
KLX02	1090.00	1096.20	2722	931216		**<0.001**	**<0.01**	**<0.01**	**1.1±0.2**	~-170 (-287)	-2.20	7.6	-78.6	-11.7	0.16	<DL	0.28	3320	151	
												18	-79.7	-11.8						
KLX02	1420.00	1705.00	2723	931222		**<0.001**					2.91							6520	140	0.46
KLX02	1420.00	1705.00	2724	931228		**<0.001**	**<0.01**	**<0.01**	**1.4±0.2**		4.86							8400	120	
KLX02	1420.00	1705.00	2725	940104							0.59							8550	120	
KLX02	1420.00	1705.00	2726	940104							0.76							8220	128	0.18
KLX02	1420.00	1705.00	2727	940111		**<0.001**	**<0.01**	**<0.01**			0.21							8780	135	
KLX02	1420.00	1705.00	2728	940112							0.69							8940	137	
KLX02	1420.00	1705.00	2729	940113		**<0.001**	**<0.01**	**<0.01**			-0.15							8830	135	
KLX02	1420.00	1705.00	2730	940114							-0.32							9020	135	0.16
KLX02	1420.00	1705.00	2731	940117	**1.0**	**<0.001**	**<0.01**	**<0.01**	**0.9±0.2**	~-300 (-334)	-0.72	26	-47.4	-8.9	0.16	<DL	0.16	9160	138	0.14
												35	-48.9	-8.8						
KLX02	1420.00	1705.00	2732	940118							-1.45							9170	126	

Bold values = risk of lower quality. Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section, SNO = Sample number, DATE = Sampling date, COND = Manual measurement of electrical conductivity in the laboratory, WFLOW = Water flow rate, DRILLW = Drilling water residue. * = The very saline groundwater and the low DOC causes high uncertainty. The error is estimated from the appearance of the analysis curves. ** = Eh values estimated from the CHEMMAC measurements. The given Eh values do not represent the true redox potential in the groundwater. In most of the cases the measuring period was to short. The values given within parenthesis represents calculated Eh values according to Grenthe et al. (1992).
*** = Repeated tritium determinations confirm the values accuracy. The reported values are recalculated from Bq/L using the relation 1 Bq = 8.45 TU.

Table 3-4: Continued. Results of trace element analyses of the samples collected using the SKB-packer sampler (µg/L). The grey marked fields indicate the most representative trace element analyses.

IDCODE	SECUP (m)	SECLOW (m)	SNO	LAB	DATE	U	Th	Y	La	Rb	Mo	Cs	Ba	As
KLX02	315.00	321.50	2738	ACT LABS	940210	1.09	0.14	0.25	0.73	5.54	19.4	0.25	43.97	17.1
				SGAB							8.0		53.0	<30
KLX02	335.00	340.80	2705	ACT LABS	931108	0.47	0.34	0.17	0.44	5.92	20.7	0.29	59.26	20.9
				SGAB							6.0		66.0	<30
KLX02	798.00	803.5	2712	ACT LABS	931123	0.76	0.16	0.11	0.02	9.83	28.4	0.52	93.40	23.4
				SGAB							7.0		105	<30
KLX02	1090.00	1096.20	2722	ACT LABS	931216	0.02	0.21	0.62	0.04	96.03	190.1	4.71	101.6	538.3
			2720	SGAB	931214						58.0		130	<300
KLX02	1420.00	1705.00	2731	ACT LABS	940117	0.02	0.28	1.82	0.36	267.67	167.3	20.03	426.91	2906.1
			2732	SGAB	940118						<50		450	<300

Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section, DATE = Sampling date, LAB = Consulted laboratory.

Table 3-5: Methods, laboratories and detection limits for the routine analysis.

Element	Method	Laboratory	Detection limit
Na	ICP-AES	KTH, SGAB*, ACTLABS*	0.04****
Ca	ICP-AES	KTH, SGAB*, ACTLABS*	0.006****
K	ICP-AES	KTH, SGAB*, ACTLABS*	0.04****
Mg	ICP-AES	KTH, SGAB*, ACTLABS*	0.0001****
Si	ICP-AES	KTH, SGAB*, ACTLABS*	0.004****
Mn	ICP-AES	KTH, SGAB*	0.0001****
	ICP-MS	ACTLABS*	
Fe(tot)	spect. (Ferrozine)	MFL	0.005
	ICP-AES	KTH, SGAB*, ACTLABS*	0.002****
Fe(+II)	spect. (Ferrozine)	MFL	0.005
Sr	ICP-AES	KTH, SGAB*	0.0001****
	ICP-MS	ACTLABS*	
Li	ICP-AES	KTH, SGAB*	0.001****
	ICP-MS	ACTLABS*	
Cl	Titr. (SIS 028120) IC**	MFL	10
F	Pot. (SIS 028135)	MFL	0.1
	IC***	MFL	
Br	IC	MFL	0.1
	Neutron activation	Studsvik AB*	
	ICP-MS	ACTLABS*	
HCO3	Titr. (SIS 028139)	MFL	0.5
S^{2-}	Spect. (SIS 028115)	MFL	0.01
SO_4	IC	MFL	0.05
SO_4-S	ICP-AES	KTH, SGAB*	0.02****
PO_4-P	Spect. (SIS 028126)	MFL	0.002
NO_2-N	Spect. (SIS 028132)	MFL	0.001
NH_4-N	Spect. (SIS 028134)	MFL	0.005
DOC	High temp. catalytic combustion Shimadzu TOC - 5000	Marin kemi	0.2

* = Control analyses, one sample per sampled borehole section.
** = Method used for concentrations < 10 mg/l.
*** = Method sometimes used for high concentrations as a control.
**** = Detection limit, ICP-AES method at KTH.

Table 3-6: Methods, consulted laboratories and detection limits for trace element and other special analysis.

Element	Method	Laboratory	Detection limit
U	ICP-MS	ACTLABS	0.01 µm/L
Th	ICP-MS	ACTLABS	0.02 µm/L
^{234}U	Alfa Spectrometry	Radiofysik, Lund	
^{235}U	Alfa Spectrometry	Radiofysik, Lund	
^{238}U	Alfa Spectrometry	Radiofysik, Lund	
^{3}H	Natural Decay counting	Energiteknikk, Kjeller	4.2 TU
	Gas counting, Propane after enrichment	GSF-Institut, Neuherberg*	0.2 TU
^{2}H	Mass Spectrometry	Energiteknikk, Kjeller	
^{18}O	Mass Spectrometry	Energiteknikk, Kjeller	
Trace elements	ICP-MS	ACTLABS	
	ICP-AES (a few elements)	SGAB	

* = Determination performed only on some samples from the first sampling occasion, tube sampling.

Laboratories:

MFL	SKB Mobile Field Laboratory
KTH	Royal Institute of Technology, Department of Chemistry, Inorganic Chemistry
SGAB	Svensk GrundämnesAnalys AB, Luleå
ACTLABS	Activation Laboratories LTD, Ontario, Canada
Studsvik AB	Studsvik AB, Nyköping
Marin kemi	Umeå Marina Forskningscentrum, Marin kemi, Norrbyn, Hörnefors
Radiofysik, Lund	Radiation Physics Department, Lund University
Energiteknikk, Kjeller	Institutt for Energiteknikk, Kjeller, Norway
GSF-Institut, Neuherberg	GSF- Institut für Hyrologie, Neuherberg, Germany

Methods:

ICP-AES	Inductively-Coupled Plasma Atomic Emission Spectrometry
ICP-MS	Inductively-Coupled Plasma Mass Spectrometry
IC	Ion Chromatography
Titr.	Titrimetric Method
Spect.	Spectrophotometric Method
Pot.	Potentiometric Measurement
Gas counting etc.	Gas counting of propane after twentyfold electrolytic enrichment of tritium

3.3.2 Quality control and comments

To ensure data quality, control analyses by independent laboratories were carried out on one sample at each sampled section. This sample was taken at the end of the pumping period using the SKB-packer sampler. Similar control analyses were performed on the third or fourth tube sample. The results of the control analyses conducted by different laboratories are given in Table 3-7. Generally the concentration of each controlled component agrees to within 10% between the various laboratories, although this is to a large extent dependent on the element in question and its concentration. If a large disparity was noted, the analyses were repeated. When the analytical sets from different laboratories were considered to be in good agreement, the data were compiled and further evaluated to produce the final dataset for each sample. The dataset given in this report is accessible through the SKB geodatabase GEOTAB. A schematic presentation of the data flow from the field to GEOTAB is shown in Figure 3-5. Detailed information of the data handling routines is given in a comprehensive report by Laurent et al. (1992).

Table 3-7: Comparison of control analyses (mg/L) between different laboratories.

IDCODE	SECUP (m)	SECLOW (m)	SNO	DATE	LAB	Na	K	Ca	Mg	SO_4-S	Br	Si	Fe	Mn	Li	Sr	P
KLX02	315.00	321.50	2738	940210	ACT LABS	126	<5.0	27	4.8		0.65	7.3	1.20	0.15	0.03	0.30	<0.05
KLX02	315.00	321.50	2738	940210	KTH	111	3.1	24	4.6	20		7.0	1.06	0.15	0.01	0.23	
KLX02	315.00	321.50	2738	940210	SGAB	117	3.4	27	4.7	18		6.8	1.11	0.16	0.02	0.27	0.046
KLX02	315.00	321.50	2738	940210	MFL					(14)	0.23		1.05				0.03
KLX02	335.00	340.80	2705	931108	ACT LABS	226	<5.0	39	6.2		1.31	6.5	0.500	0.15	0.04	0.49	<0.05
KLX02	335.00	340.80	2705	931108	KTH	206	3.1	36	5.9	29		6.4	0.465	0.14	0.03	0.39	
KLX02	335.00	340.80	2705	931108	SGAB	209	2.9	39	6.1	29		6.0	0.489	0.14	0.03	0.50	0.048
KLX02	335.00	340.80	2705	931108	MFL					(28)	0.67		0.464				
KLX02	798.00	803.80	2712	931123	ACT LABS	298	<5.0	124	10.5		4.09	7.5	1.95	0.55	0.08	1.67	<0.05
KLX02	798.00	803.80	2712	931123	KTH	288	4.5	123	10.6	37		7.5	1.83	0.39	0.08	1.66	
KLX02	798.00	803.80	2712	931123	SGAB	286	4.3	125	10.5	38		7.0	1.87	0.40	0.08	1.77	<0.04
KLX02	798.00	803.80	2712	931123	MFL					(35)	2.4		1.73				<0.01
KLX02	1090.00	1096.20	2720	931214	SGAB	3800	11.8	5580	2.4	293		4.9	<0.05	0.02	2.25	101	0.813
KLX02	1090.00	1096.20	2720	931214	KTH	3750	11.4	5670	1.9	320		5.4	<0.002	0.02	1.94	95.6	
KLX02	1090.00	1096.20	2722	931216	Studsvik						138						
KLX02	1090.00	1096.20	2720	931216	MFL					(336)	125		0.007				
KLX02	1420.00	1705.00	2731	940117	ACT LABS	8100	35.0	>range	2.6		409	4.9	0.400	0.17	6.07	309	1.00
KLX02	1420.00	1705.00	2732	940118	KTH	8010	33.0	18500	2.7	315		4.8	0.325	0.13	5.38	343	
			2731										0.405				
KLX02	1420.00	1705.00	2732	940118	SGAB	8370	54.3	18600	3.3	243		4.9	0.343	0.12	6.04	348	1.39
KLX02	1420.00	1705.00	2732	940118	Studsvik						406						
KLX02	1420.00	1705.00	2731	940117	MFL					(277)	312		0.405				
			2732										0.346				

( ) = IC determination of sulphate, recalculated to sulphur

Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section, SNO = Sample number, LAB = Consulted laboratory, DATE = Sampling date, SO_4-S = Sulphur by ICP-AES, Fe = Total Iron by ICP-AES.

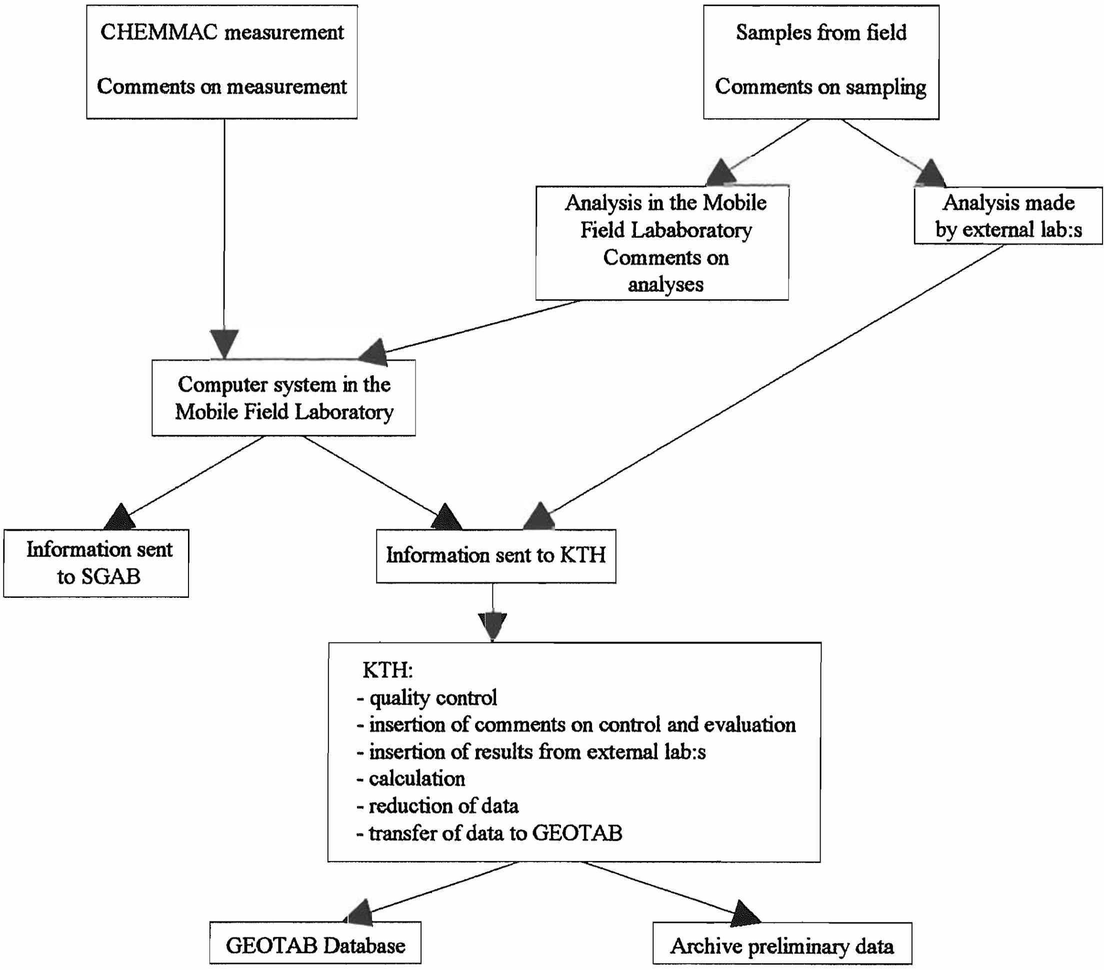


Figure 3-5: *A schematic presentation of the data flow from the field to the SKB database GEOTAB (modified after Laurent et al. 1992).*

Charge balance errors indicate the quality of the major components analysed. The relative charge balance errors for the samples from KLX02 never exceed 5% which is considered acceptable. The expression for the relative charge balance error is given below (Eq#1):

$$\text{Rel. Charge Balance Error} = \frac{(\text{equivalents of cations/l} - \text{equivalents of anions/l})}{(\text{equivalents of cations/l} + \text{equivalents of anions/l})}$$

The very saline groundwater in the two deep borehole section caused analytical problems for some methods and some of the components. The questionable elements are marked with **bold** in the presented dataset. Further details and comments on certain determinations are given below:

- Potassium, and silicon are difficult elements to resolve using ICP-AES. The agreement in Table 3-7 is considered acceptable.

- Sulphate is determined by ion chromatography and as sulphur by ICP-AES. Differences of up to 26% between the highest and the lowest concentration values are recorded in Table 3-7. Table 3-4 shows a fairly large scatter of IC determinations which contrasts with almost constant ICP values (KTH). This indicates that the ICP values (SO_4-S) are more reliable.

- Bromide. Repeated determinations will be performed by Studsvik; their results agree with ACTLABS if multiplied by 10 as in Table 3-7. Perfect bromide peaks were obtained by ion chromatography in the field laboratory. As an old standard solution is suspected to have caused the lower bromide values by IC, the standard is going to be checked.

- Phosphate, nitrite, and ammonium. The standard methods used in the field laboratory were less reliable because of the very concentrated nature of the waters in the two deep sections. For phosphorus the ICP results are reported; confidence in the ammonium results are also limited.

- DOC. The highly saline groundwaters and the low DOC causes a high degree of uncertainty. An error of ± 0.2 mg/l was estimated from the shape of the analyses curves.

- Eh given in Table 3-4 are estimated values from those recorded at the end of the measuring periods; all electrodes are taken into consideration even if they do not agree. Note that the Eh values given do not necessarily represent the true redox potentials in the groundwater. In most cases they show that the measuring period was too short or, in one case, that the redox potentials were difficult to measure due to low iron concentrations in the water (KLX02:1090-1096.2 m). Within parenthesis, calculated Eh values according to Grenthe et al. (1992) are included for comparison. The calculated values show a range from -287 to -387 mV compared with the measured -40 to -300 mV which indicate that the electrodes had inadequate time to reach a stable level.

- Uranium. The level and the trend of the uranium concentrations are more or less confirmed by comparing recalculated ^{238}U isotope values (mBq/l) and uranium by ICP-MS in µg/l. The ICP-MS values are always higher by a factor of 1.7-3.3 times.

- Trace elements. The risk of contamination is obvious from the pump and other instrumentation in the borehole; the contact between water and metal cannot be avoided. The elements that were considered excellent or good in the report by Wikström and Björklund (1994) are also reported here together with thorium and arsenic.

3.4 Representativeness of groundwater samples

Groundwater hydrogeochemical data often comprise a large number of variables, all of which contribute a particular piece of information. The history, reactions, mixing situations and the flow paths of the groundwater may be coded in these variables. In order to make best use of these variables the quality of the field and laboratory data must be ensured as the understanding of natural groundwater systems is no better than the data on which they are based.

The importance of groundwater quality for the interpretation of deep groundwater chemical components cannot be overstressed. For example, the main constituents, Na, K, Ca, Mg, Cl, HCO_3 and SO_4 indicate the groundwater residence time in the rock by showing the extent of the rock/water interaction. Elements such as F, Br, PO_4 and SiO_2 are useful for identifying the origin of the water and the state of equilibrium. Fe(II), Fe(tot) and S(-II) are primarily analysed in order to describe the redox conditions and thus to support the Eh measurements. They also give information on the buffer capacity of the water.

By definition *a high quality sample is considered that which best reflects the undisturbed hydrological and geochemical in situ conditions for the sampled section.* A low quality and hence unrepresentative sample reflects in situ, on-line, at-line, on-site or off-site errors such as excessively high and low extraction pump-rates, contamination from borehole activities, complex hydrological situations, contamination from tubes of varying compositions, air contamination, losses or uptake of CO_2, long storage times prior to analyses, analytical errors etc. The quality may also be influenced by the rationale in locating the borehole and selecting of the sampling points. Some errors are easily avoidable, others difficult or impossible. Furthermore, chemical responses to these influences are sometimes apparent, but not always (Laaksoharju et al., 1993).

Groundwater quality evaluations have been carried out at the Äspö Hard Rock Laboratory site (Smellie and Laaksoharju, 1992). The sequence of activities from drilling to groundwater sampling was not always systematic; groundwater sampling (sometimes only limited to uranine tracer monitoring of the flushing water contents) were carried out at various occasions in association with drilling, borehole clearance and pump tests etc. At Äspö, drilling and hydraulic testing using near-surface waters (<100 m) may have resulted in direct contamination.

At Laxemar the focus was on avoiding interference from drilling, hydrotesting and other borehole activities. Open-hole conditions, however, may have contributed to a general mixing of groundwater types in the borehole; the degree of mixing will depend on the hydraulic properties of the borehole and possibly on groundwater density variations. In Laxemar this risk is considered to be large since the upper part of the borehole may represent active recharge. Subsequent raising and lowering of geophysical probes and tube sampling may also have caused groundwater perturbation in the boreholes resulting in the mixing of non-saline and saline water types. Furthermore, it is a known phenomenon for groundwaters to undergo significant pH and Eh changes through degassing and oxidation etc. when slowly pumped the long distances to the surface (transport time 5-6 h for the shallower sections and 10-12 h for the two deepest sections); this is believed to be a significant problem in deep boreholes such as Laxemar.

To minimise possible contamination and/or exchange reactions (and also to remove microbes) on the inner diameter surface of tube leading sampled water to the surface, a new routine was adapted when sampling using the SKB-packer equipment. The whole water tube was cleaned after every sampled section by using hypochloride. This resulted in a black out-wash of which 250 mL was filtered on a 450 nm polycabonate filter and sent for analyses. The Al, Si, S, Ca, Mn, Fe and Ba contents were determined using energy dispersive XRF (X-ray fluorescence). The element values from the filter analyses (in ppb) showed; Al = 37.3, Si = 1245, S = 1259, Ca = 1948, Mn = 40, Fe = 3722 and Ba = 586. These particles may form mineral phases in equilibrium with the present water e.g. $BaSO_4$ (barite) and FeS_2 (pyrite). This equilibrium may smooth out or even change many of the in-situ element values obtained since the water is up to 12 h in contact with these particles in the water tube.

Most of the samples were, as planned, collected at low extraction rates (<200 mL/min) in order to minimise contamination. In general, careful planning and other precautionary measures such as long sampling times have provided a reasonable degree of confidence in the representativeness of the samples. This is supported by the on-line monitoring data with the CHEMMAC sond. On-line CHEMMAC measurements were carried out at each borehole section to ensure that a stable chemical environment had been achieved prior to sampling. Depending on earlier drilling activities and borehole hydraulics, chemical stability of the groundwaters being monitored may be achieved after a few hours, but equally it may take days or even weeks. This stage of the programme is critical in order to ensure representative sampling.

Continuous computer controlled on-line measurements were performed by two different parts of the SKB mobile field laboratory equipment. One part, the so-called Borehole CHEMMAC, is a down-hole probe for in situ measurements in the borehole section. This was located in the sampled borehole section (between the upper and lower packer) except for the two deep sections were the system was modified according to Figure 3-3. The other part of equipment, the Surface CHEMMAC, is a measuring cell housed in the laboratory unit on the surface. The pumped water passes the measuring cell on its way to the outlet. Both sets of equipment measure pH, redox potential and temperature; electrical conductivity and dissolved oxygen is measured by the Surface CHEMMAC. Measurement of the on-line temperature, pH, electrical conductivity and Eh are presented as plotted curves for the five sampled borehole sections in the Figures 3-6a,b,c,d and e. Important borehole activities and technical problems which have affected the sensitive measurements of Eh and pH are also shown. The sensitivity of these important parameters to disturbance illustrates the problems encountered when sampling for deep groundwaters (Wikberg, 1987).

Figures 3-6a,b,c,d and e show the occasion when sampling was carried out; in most cases a stable groundwater chemistry was indicated at this juncture. The only section where the electrical conductivity values are still changing is the 798-803.8 m level; this section should have been sampled for a longer period of time. Technical problems mostly due to packer problems occurred at every section except at the deepest 1420-1705 m level. This resulted in maintenance uplifting of the equipment such that possible leakages around the packers may have caused perturbation and mixing of water. This could have resulted in an influx of brackish waters into the borehole above the packer system, originating from hydraulically conducting fracture zones intersecting the borehole at shallower depths (e.g. 220 m). Degrees of mixing of younger groundwaters (i.e. less than 30 years) is indicated by the tritium contents which are all in excess of 4.2 TU (detection limit). This would suggest that even though chemical stability of the groundwaters was achieved prior to sampling, evidence of mixing which occurred at an earlier stage in the history of the borehole is still apparent, even down to the deepest levels. Contamination by drilling water can be ruled out as uranine contents are consistently less than 1%.

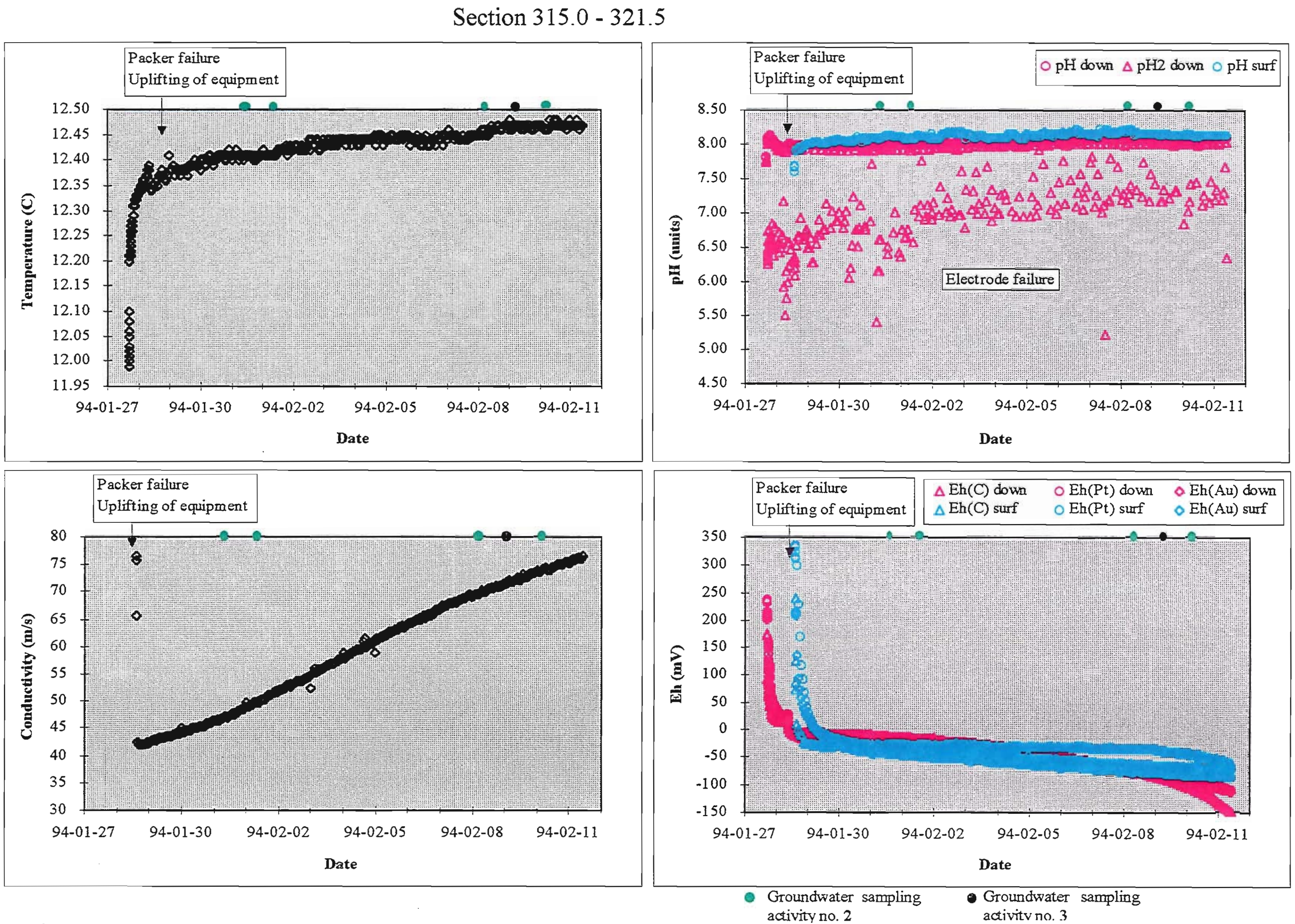


***Figure 3-6a:** SKB-packer sampling (section 315-321.5m); downhole and surface on-line CHEMMAC results: Temperature, pH, electrical conductivity and Eh records versus sampling date are shown. Important borehole activities and technical problems which have affected the measurements are also indicated. Green dot = complete chemical sampling (groundwater sampling activity no 2 in Table 3-1); black dot = less extensive chemical sampling (groundwater sampling activity no 3 in Table 3-1).*

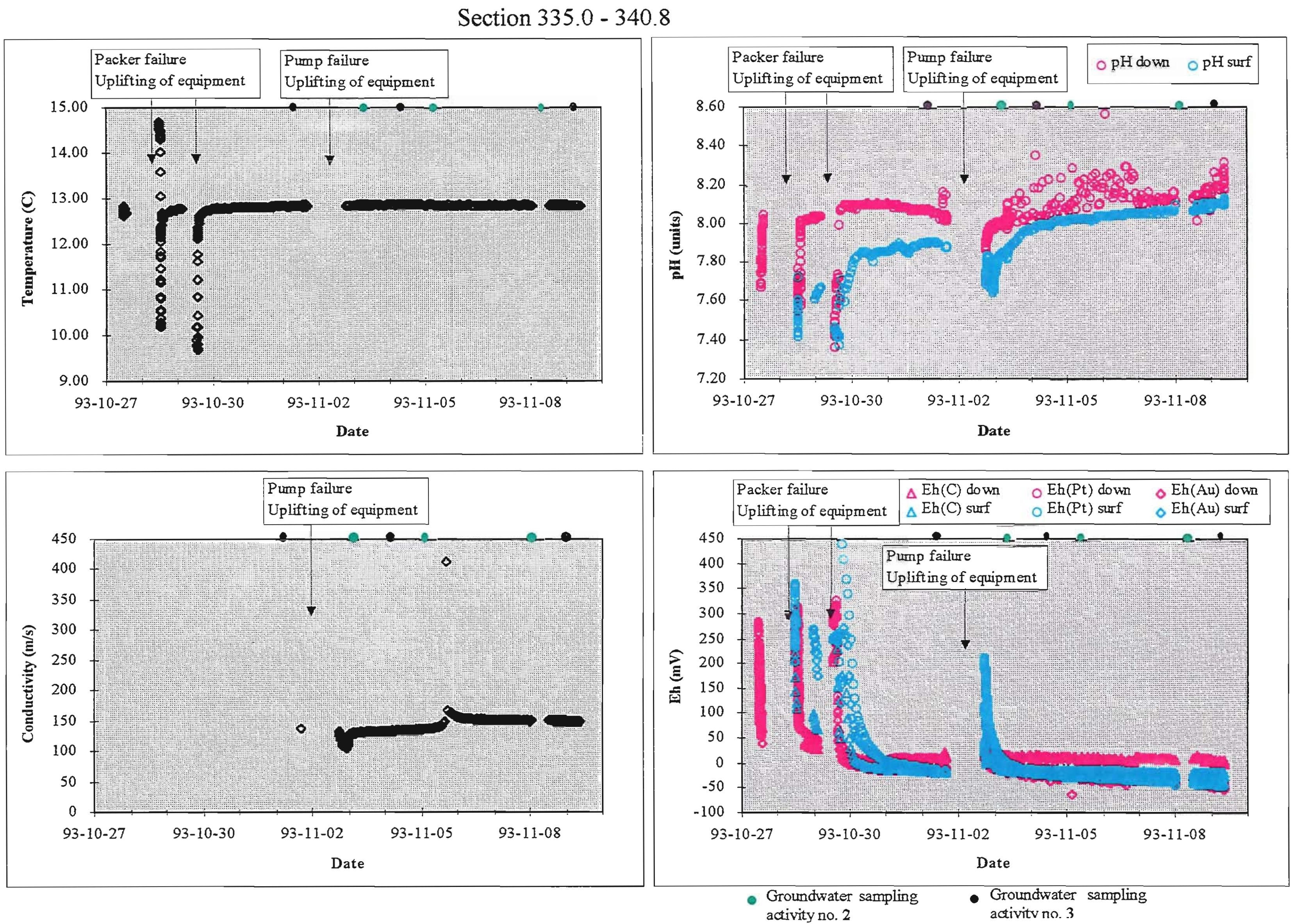


Figure 3-6b: *SKB-packer sampling (section 335-340.8m); downhole and surface on-line CHEMMAC results: Temperature, pH, electrical conductivity and Eh records versus sampling date are shown. Important borehole activities and technical problems which have affected the measurements are also indicated. Green dot = complete chemical sampling (groundwater sampling activity no 2 in Table 3-1); black dot = less extensive chemical sampling (groundwater sampling activity no 3 in Table 3-1).*

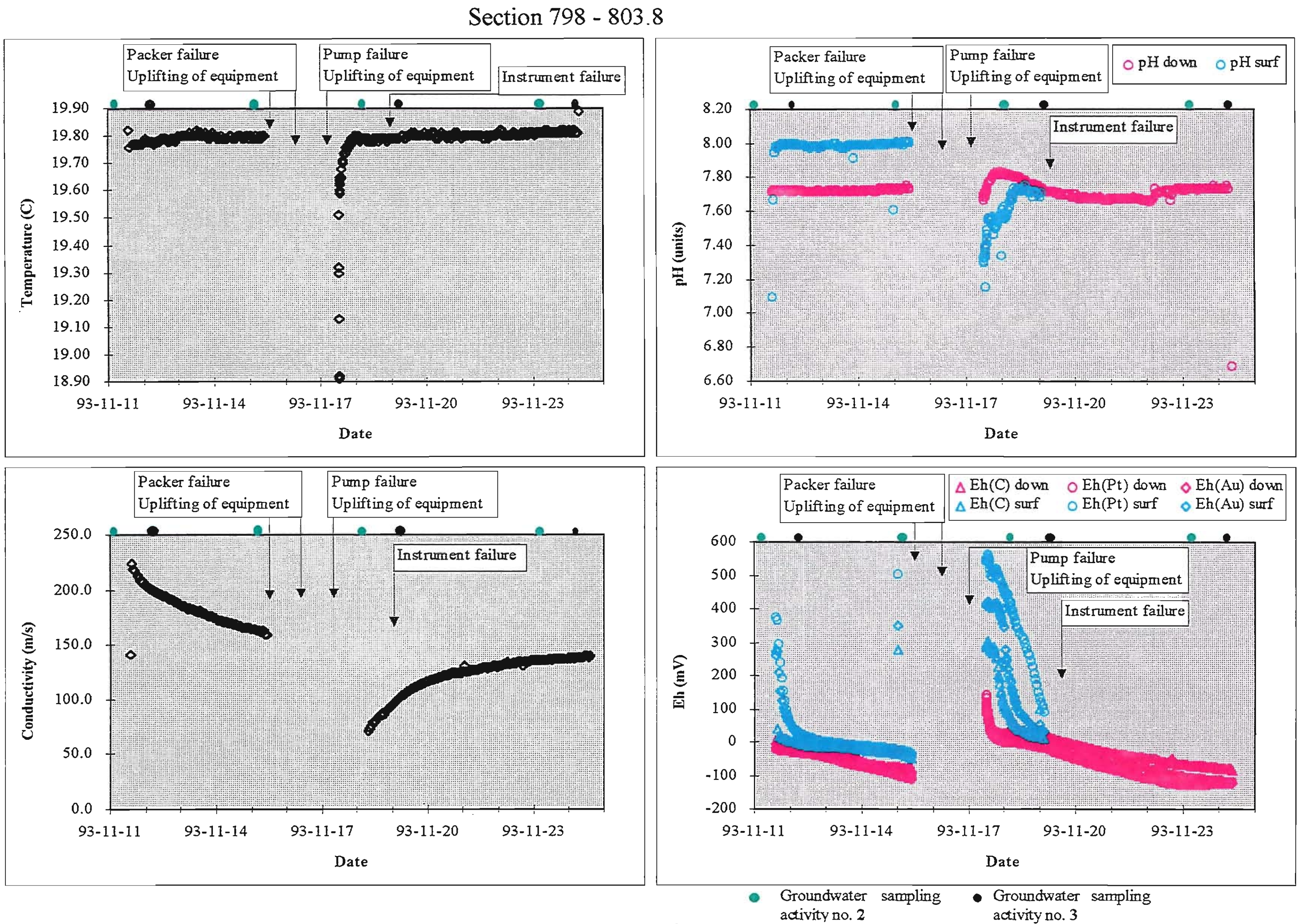


Figure 3-6c: *SKB-packer sampling (section 798-803.8m); downhole and surface on-line CHEMMAC results: Temperature, pH, electrical conductivity and Eh records versus sampling date are shown. Important borehole activities and technical problems which have affected the measurements are also indicated. Green dot = complete chemical sampling (groundwater sampling activity no 2 in Table 3-1); black dot = less extensive chemical sampling (groundwater sampling activity no 3 in Table 3-1).*

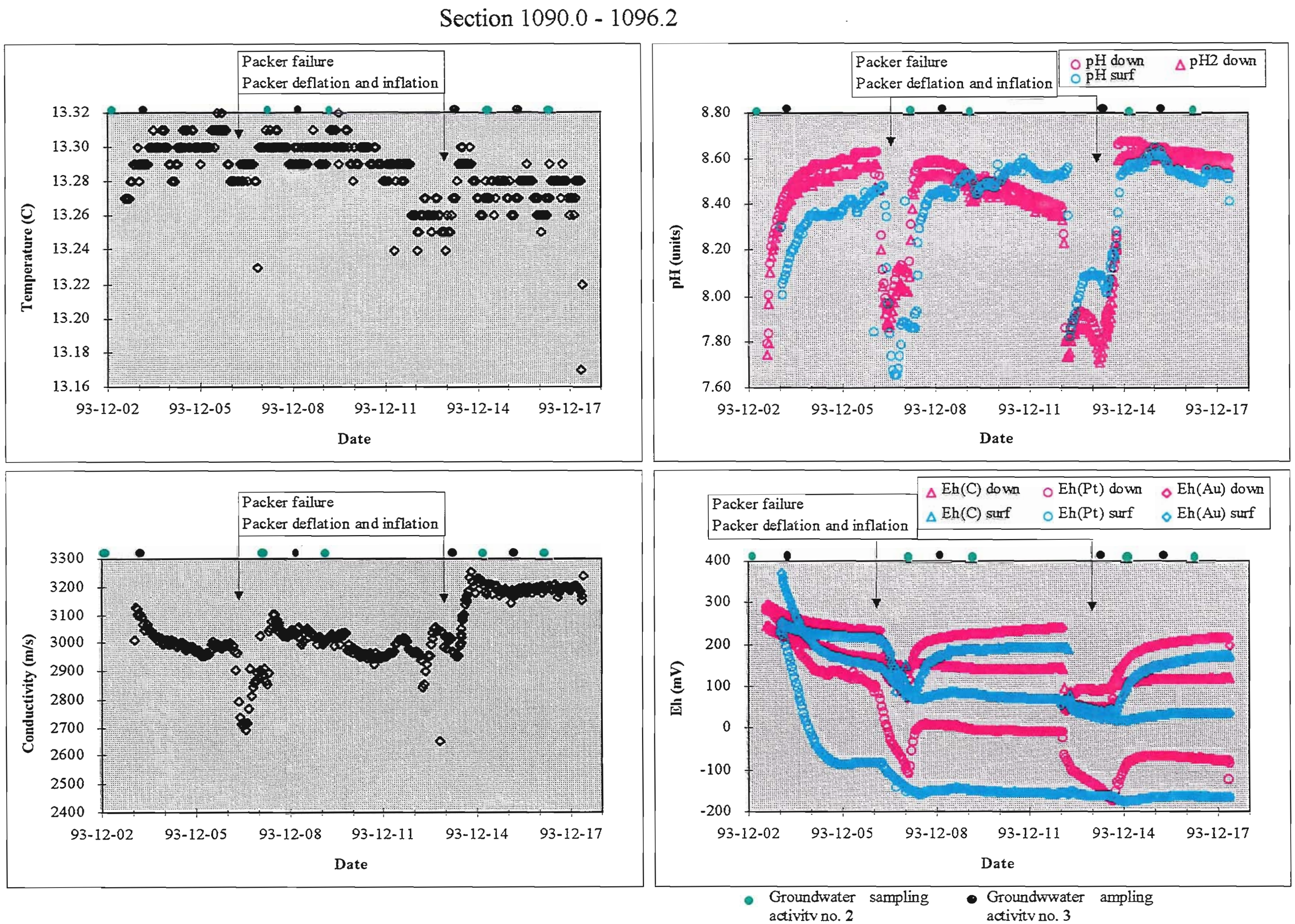


Figure 3-6d: *SKB-packer sampling (section 1090-1096.2m); downhole and surface on-line CHEMMAC results: Temperature, pH, electrical conductivity and Eh records versus sampling date are shown. Important borehole activities and technical problems which have affected the measurements are also indicated. Green dot = complete chemical sampling (groundwater sampling activity no 2 in Table 3-1); black dot = less extensive chemical sampling (groundwater sampling activity no 3 in Table 3-1).*

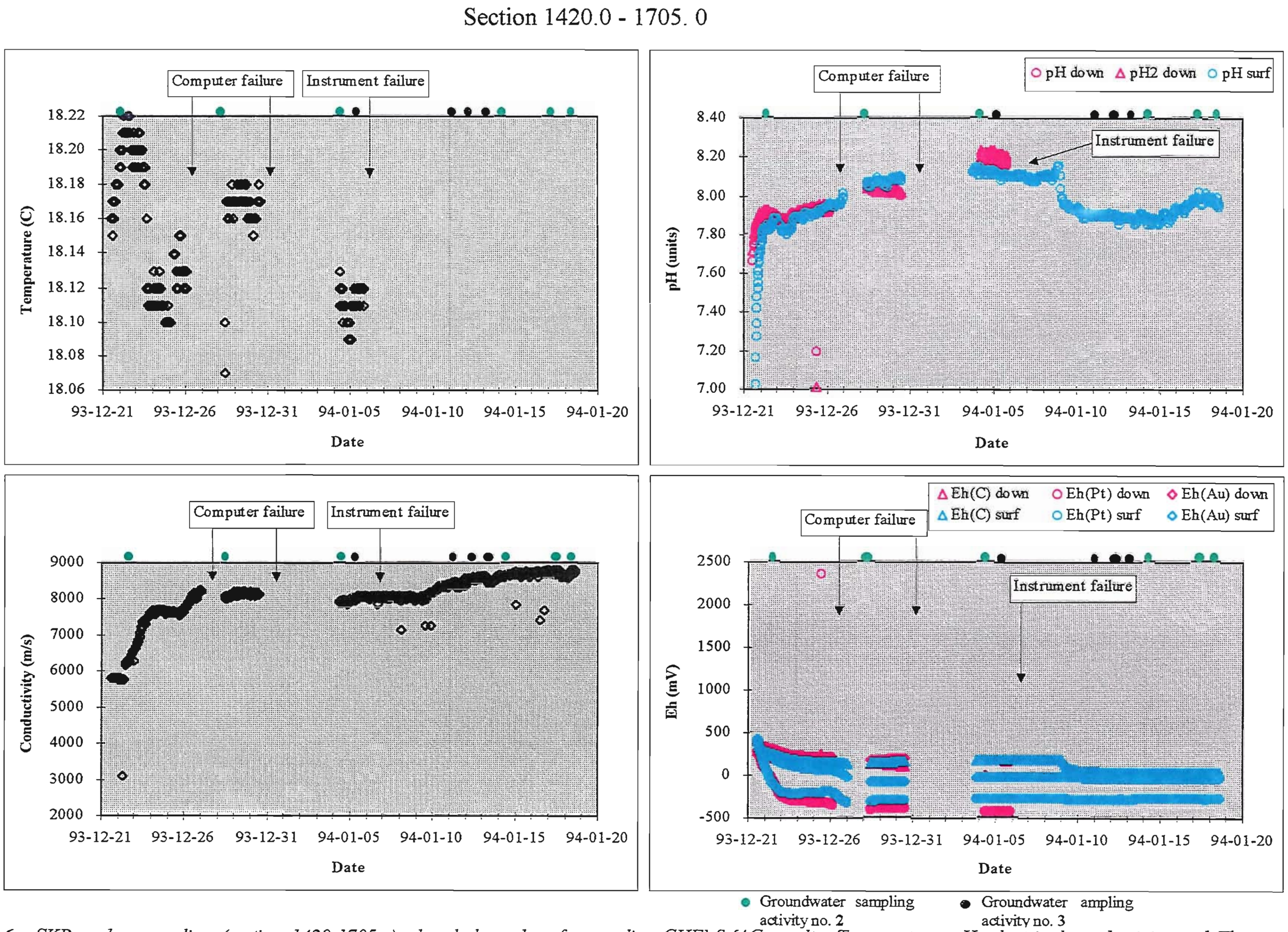

Section 1420.0 - 1705. 0

Figure 3-6e: *SKB-packer sampling (section 1420-1705m); downhole and surface on-line CHEMMAC results: Temperature, pH, electrical conductivity and Eh records versus sampling date are shown. Important borehole activities and technical problems which have affected the measurements are also indicated. Green dot = complete chemical sampling (groundwater sampling activity no 2 in Table 3-1); black dot = less extensive chemical sampling (groundwater sampling activity no 3 in Table 3-1).*

Of particular interest is the high recorded amount of tritium (26 TU) from the 1420-1705 m section which, at face value, indicates the presence of substantially high quantities of modern (i.e. present-day) recharge water. However, this explanation is inadequate since the tritium value is higher than present-day precipitation levels which lie around 22 TU. Since in-situ production of tritium may be ruled out because of a complete absence of uranium mineralisation in the host rock, the only remaining possibility involves natural or artificial (i.e. drilling; hydrotest during drilling; open-hole effects; pumping) groundwater mixing processes (see section 3.5.3). In conclusion, artificial mixing processes appear to be the most plausible explanation at the moment for the recorded tritium values, and some doubt may therefore exists as to the total representativeness of the samples from the borehole. The contamination, which shows low saline water entering at large depths (Figure 3-7), may have occurred when the hydrotests were carried out during drilling.

Generally, samples taken with the Tube sampler might be considered of lower quality when compared with the SKB double packer sampling system. Interestingly this is not the case (except for the pH values); comparison with most elements indicate a surprisingly similar character although somewhat more dilute i.e. less saline Cl^- concentration, characterises the Tube sampler method. Consequently, these data have been incorporated in this present evaluation. Using the conservative ion chloride, Figure 3-7 compares the results of both sampling methods; drilling water data are also included. A strong dilution of the borehole water has taken place during drilling. This may have introduced mixing of foreign water types. There is a close correlation of chloride variation between the tube and packer methods, even though a greater dilution would have been expected from the Tube sampler method as this was carried out under open-hole conditions. It is only at the 1100 m and 1600 m level that greater salinity is recorded using the SKB-packer sampling method. These data provide an interesting insight into the hydraulics of the borehole and host bedrock.

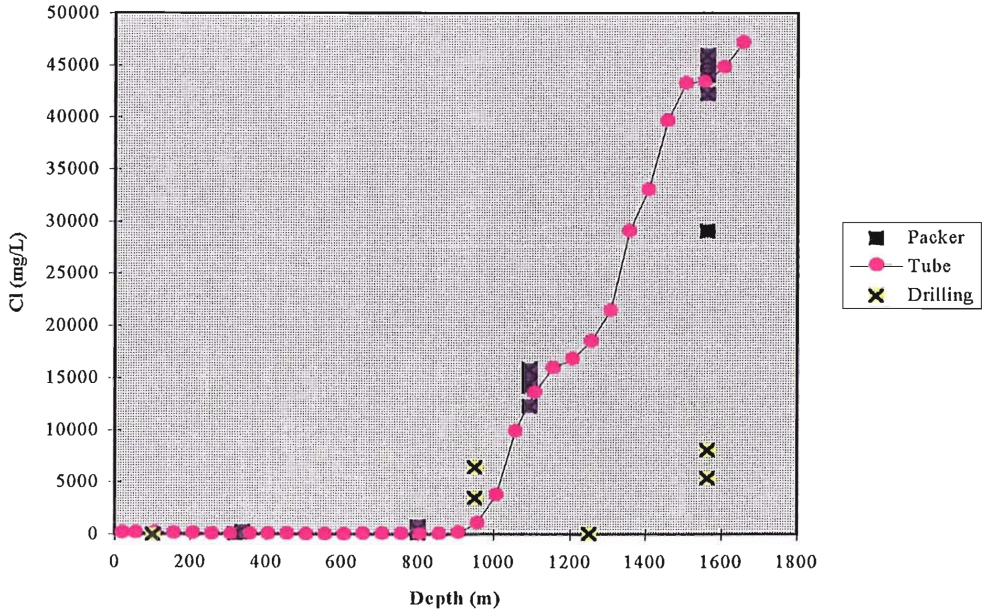


Figure 3-7: *Cl concentrations in groundwaters sampled in KLX02 during; hydrotests during Drilling, Tube sampling, SKB-Packer sampling.*

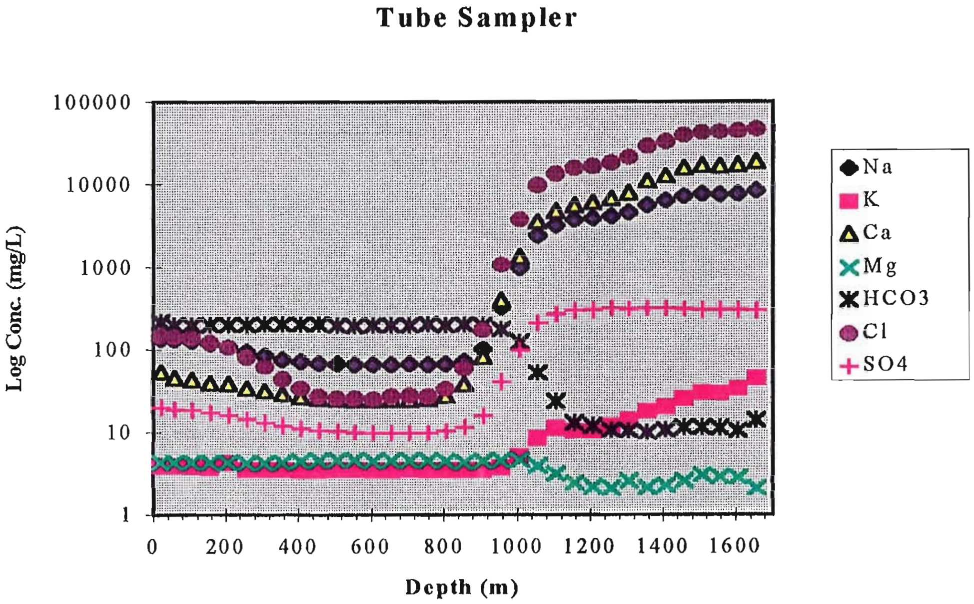
Bearing in mind that groundwater mixing to varying degrees is apparent at all sampled levels, the most "representative" samples collected from KLX02 using the SKB-packer sampler system are shaded grey in Table 3-4. These have been selected on the basis of monitoring data from CHEMMAC (Figures 3-6a,b,c,d, and e) and their chemistry to be the most suitable for further modelling work.

3.5 Groundwater chemistry

3.5.1 Description and classification

Groundwater analyses of KLX02 are presented in Tables 3-3 and 3-4; major ion depth trends are illustrated in Figure 3-8. The sharp break in the Cl composition at around or after 900 m, indicated by both sampling methods, is reflected by all other major elements in Figure 3-8. The plots show that the dominating ions in the shallow water are in descending order; HCO_3, Na, Cl and Ca and the deep water Cl, Ca, Na and SO_4. Increases with increasing depth are shown by Na, Ca, K and SO_4 with sympathetic decreases in Mg and HCO_3. Shown in Appendices 1 and 2 (matrix scatter plots) are increases in Br, Li and Sr and decreases in F, Si and Fe.

A)



B)

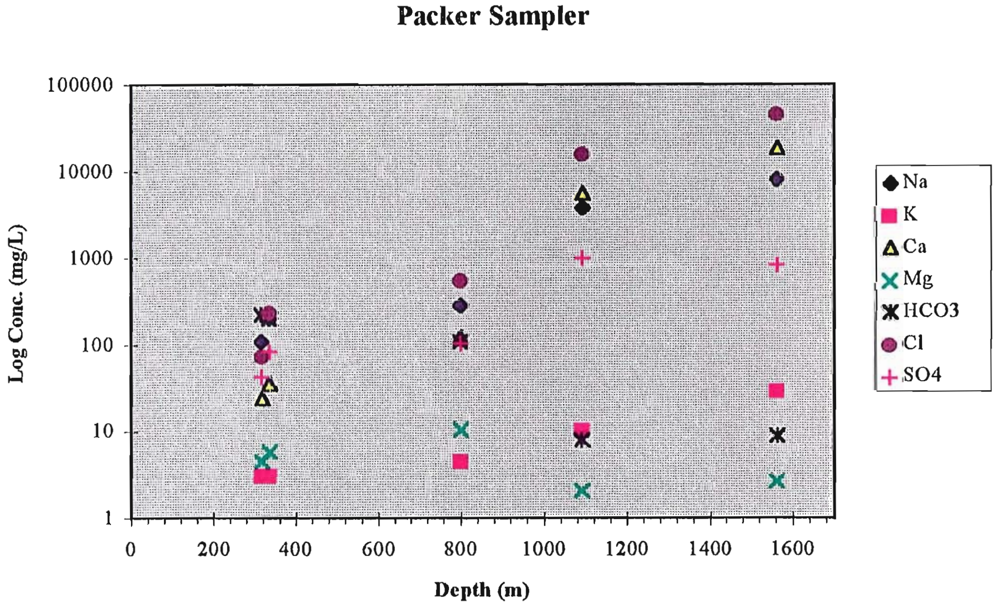


Figure 3-8: *Borehole KLX02: Groundwater major ion depth trends using A) Tube sampler (open-hole water), and B) SKB-packer sampler system (fracture water).*

Piper plots (Piper, 1953) are widely used to present and classify major ion groundwater data. To compare the Laxemar data with the Äspö groundwaters standard trilinear Piper Plots were used based on Davis and De Wiest (1967). The major variables used were Cl, Na, Ca, HCO_3, Mg, K and SO_4. The GEOTAB database contains samples from Äspö, the Redox Zone, Ävrö, Laxemar, Baltic sea and samples taken along the access tunnel to the Hard Rock Laboratory at Äspö (HRL) (Figure 1-1). The samples were divided into three groups: shallow, intermediate and deep according to: **Shallow** = 0-1000 mg/L Cl, **Intermediate** = 1000-6500 mg/l Cl and **Deep** = > 6500 mg/L Cl. The samples from the Baltic sea were named **Sea**; the pore water extracted from the sea sediments close to Äspö (SAS48) were named **Sediment**. The samples from the Redox Zone were named **Redox**. In addition, a classification system developed by Morgan and Winner (1962) and Back (1966) was included in the plot. The water types are designated according to the domain in which they occur on the diagram segments (Figure 3-9).

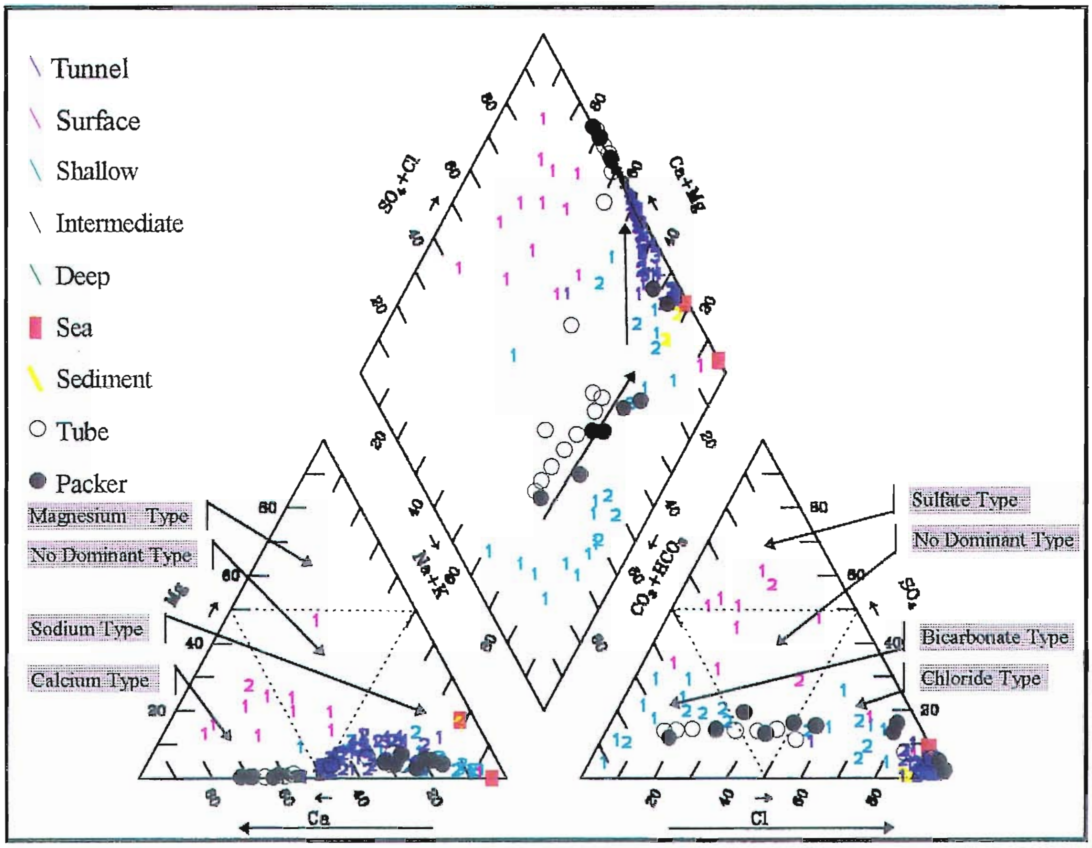


Figure 3-9: Standard Piper Plot showing the main groundwater types for the Äspö area in relation to the Laxemar samples taken with the Tube sampler and the SKB-packer sampler (percentage scales). Possible groundwater evolution and/or mixing trends are shown with black arrows. The waters are classified according to domain (grey tagged) in which they occur on the diagram segments.

The Piper Plot clearly demonstrates the large spread of groundwater compositions with two distinct groupings; one shallow to intermediate *Sodium-Bicarbonate* type [Na(Ca,K):HCO_3-Cl(SO_4)] and the other of deep origin a *Calcium-Chloride type* [Ca-Na(K):Cl-SO_4(Br)]. Similarities to these general groundwater patterns from Äspö have been described from two localities in Finland; from Hästholmen (Nordstrom, 1989) and more recently from Olkiluoto (Pitkänen et al., 1992). For Laxemar the plot indicates that there is an evolution and/or mixing trend from shallow water through intermediate water to the Laxemar deep water. Influence from the Baltic Sea is evident from some of the tunnel data. The disadvantage with Piper plots is the higher resolution for the more shallow waters than for the intermediate and the deep groundwaters; the latter usually forming tight clusters.

The stable isotope data (Figure 3-10) support the two major groundwater types as defined above. The shallow groundwaters ($\delta^{18}O$ = -12.1 to -9.9‰; $\delta^{2}H$ = -85.2 to -73.4‰) tend to plot close to the Global Meteoric Waterline (GMW); in contrast the deep saline varieties ($\delta^{18}O$ = -10.4 to -8.9‰; $\delta^{2}H$ = -60.2 to -44.9‰) show significant deviation from the meteoric water line. Even though there is undoubtedly mixing of less saline meteoric and highly saline groundwater types, there is a distinct trend, with increasing salinity, along a slope greater than 8. This is in accordance with the deep Canadian brines (Frape and Fritz, 1987) which show similar characteristics (e.g. Sudbury). The trend towards increasing salinity also reflects a greater dependency on water/rock reactions and increasing geothermal temperature (pers. comm. Wallin, 1995) in combination with minimal influence from past marine and glacial melt fluctuations. These palaeoclimatic variations characterise the spread of $\delta^{18}O$ values at lower salinities. The stable isotope data from Laxemar borehole KLX02 are compared with Äspö area data in Figure 3-11. It is clear that the shallower depths (0-1000 m) represented at Laxemar show similar isotopic mixing and evolutionary trends as those described for Äspö (Smellie and Laaksoharju, 1992; Smellie et al., 1995).

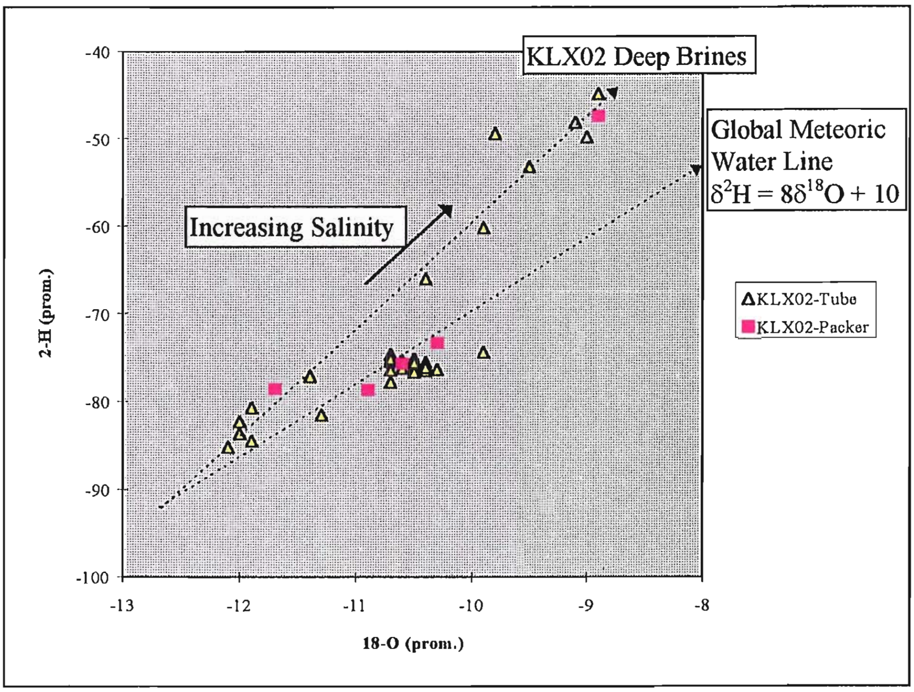


Figure 3-10: Stable isotope plot of the Laxemar data from borehole KLX02.

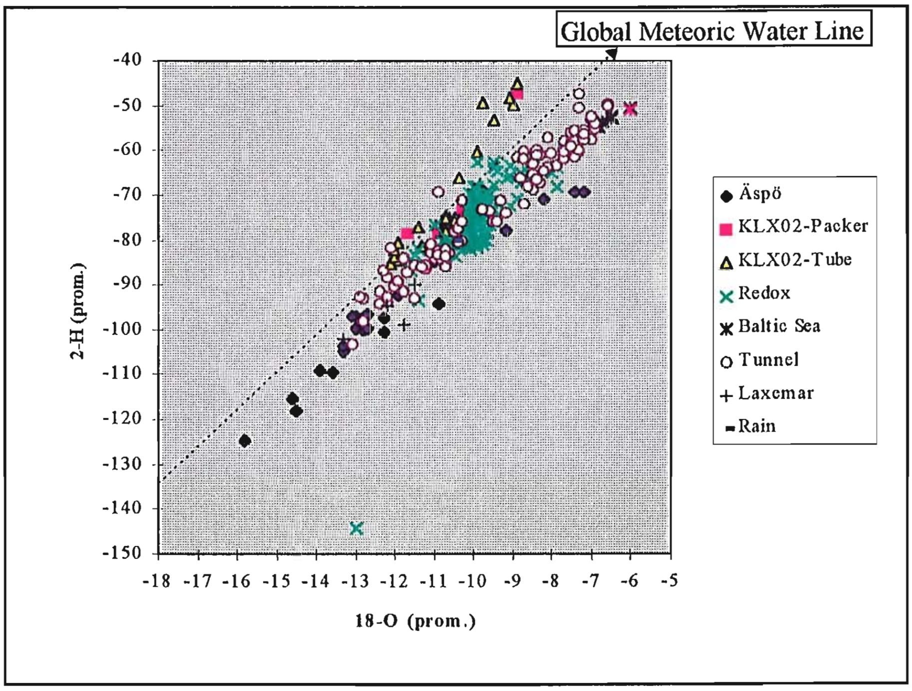


Figure 3-11: The stable isotope data from Laxemar borehole KLX02 compared with Äspö area data.

3.5.2 Evolutionary trends

To model evolutionary trends in Laxemar the samples from KLX02 were divided into two groups: Tube sampler (**KLX02-Tube**) and SKB-packer sampler (**KLX02-Packer**). These data have been compared with data from the Äspö area (data from the SKB-database GEOTAB); samples (including, Äspö, Ävrö and other Laxemar boreholes than KLX02) were named **Äspö,** samples taken from The Redox zone were named **Redox**, and samples from the Baltic sea where named **Sea**. Also included in the calculations are HRL-tunnel groundwater data named **Tunnel** (for location of the sampling places see Figure 1-1).

Principal Component Analysis (PCA) which is a form of multivariate analysis was used to illustrate the evolution and changes of the water chemistry sampled at Laxemar in relation to waters from nearby investigated sites. The strength of this approach is that several or all variables in a data matrix can be examined simultaneously. Greater resolution is possible and the character of the data in a general data matrix is therefore more easily identified than using univariate analysis, where only one variable is compared at a time (Wold, 1987). This technique has been used earlier at Äspö (Laaksoharju and Nilsson, 1989; Laaksoharju, 1990; Smellie and Laaksoharju, 1992).

The major components Cl, Ca, Na, Mg, K, SO_4 HCO_3 and ^2H, ^{18}O and ^3H from KLX02 were used. These components are known from other studies to describe most of the variability in the data and contain most of the groundwater evolution information.

PCA is focused on the variance or variability of the data. With this technique the main aim is to replace the original variables by a smaller number of "underlying" variables. New variables will hopefully give a better understanding of the data. Principal Component Analysis consists of finding an orthogonal transformation of the original variables to a new set of non-correlated variables (Chatfield and Collins, 1989). This transformation consists of a rigid rotation or a rotation plus reflection preserving the distances and angles in the matrix. The new variables are called Principal Components, which are linear combinations of the original variables. The components are derived in decreasing order of importance. Generally the first few components will account for most of the variation in the original data so that the effective dimensionality of the data can be reduced and hence the information is simplified. The results of the analyses are shown in Figure 3-12.

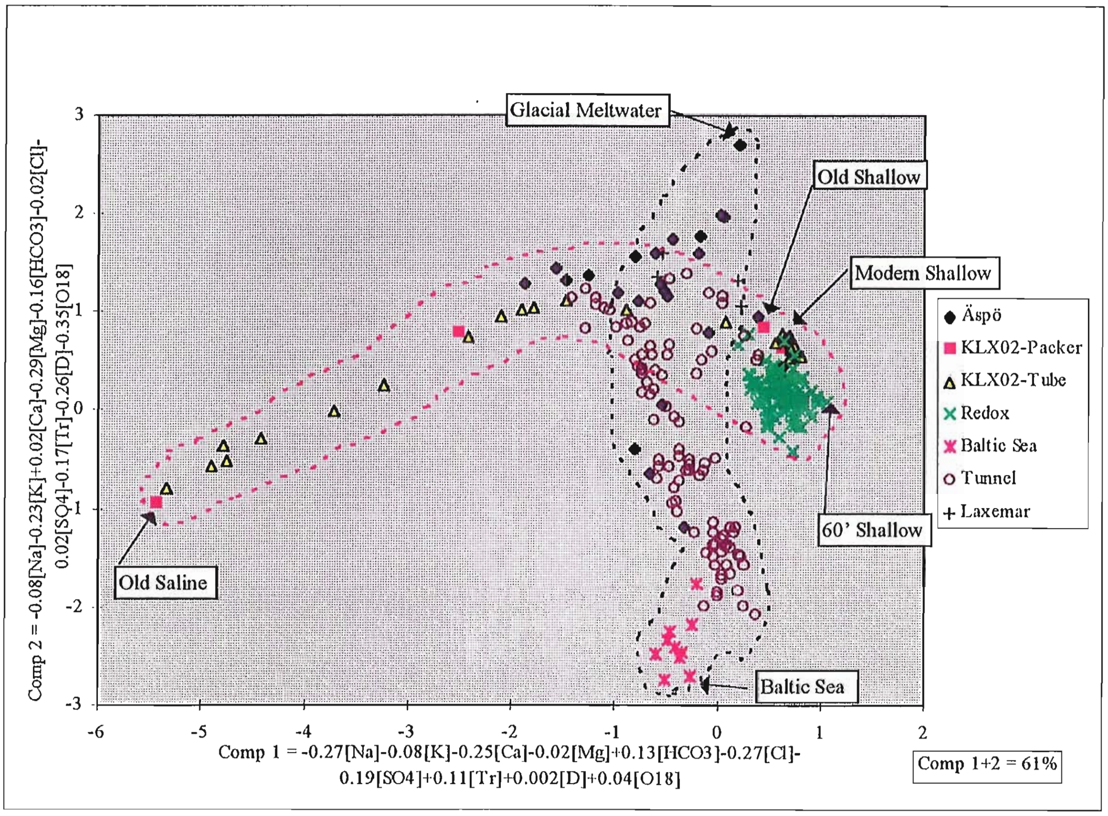


Figure 3-12: *Principal Component plot based on the major components and stable isotopes and tritium values from KLX02 in relation to the main groundwater types found in the Äspö area. The position of the selected end-members are boxed in black. Possible evolution/mixing patterns for the groundwaters are marked by dotted lines. The red dotted area represents an assumed Shallow water - Old Saline water evolution pattern and the black dotted area a Baltic Sea - Glacial meltwater evolution pattern. The respective weight for the different elements are shown in the equations for the first and the second principal component. These components together describe 61% of the variability (or the information) in the data.*

The selected end-members in Figure 3-12 represent extreme waters that are found in the Äspö area. The **Glacial Meltwater** end-member has been determined as an old glacial meltwater water based on the stable isotope values which indicate cold climate recharge (^{18}O= -15.8 SMOW and ^{2}H= -124.8 SMOW) in combination with an apparent ^{14}C age of 31 365 years (Smellie and Laaksoharju, 1992). The presence of glacial melt water as an end-member is reflected by the stable isotope data plotted in Figure 3-11 which clearly shows the Äspö glacial melt water at very light δ^{18}O values (-14 to -16‰). This type of water is found in Äspö KAS03:129-134 m. The **Old saline** water represents the brine type of water found in

KLX02:1420-1705 m, the **Baltic sea** represents modern Baltic sea water (SEA01). The Shallow waters have been selected based on a theoretical calculation where the tritium value for rain water was based on; 100 TU = water from 1960, 22 TU = water from 1994 and 0 TU = water older than 1960. The measured waters which plotted close on the PCA plot to the calculated waters, were set to represent a particular shallow water based on; **60' Shallow** water represents water from 1960 found in the Redox Zone (HBH02:7.5 m). **Modern Shallow** water represents modern shallow water found in KLX02:81-131 m (Tube sampler). **Old Shallow** water represents older than 1960 water with no or low tritium content found at Äspö KAS04:226-235 m. The determined ^{14}C age of the water gave an apparent age of 7795 years (Smellie and Laaksoharju, 1992). The selected end-members are believed to best represent waters that interact in different degrees and portions in groundwaters sampled from the whole area.

Two main evolution patterns have been identified in Figure 3-12. The red dotted area represents a assumed *Shallow water - Old Saline water* evolution pattern, the black dotted area a *Baltic Sea - Glacial meltwater* evolution pattern. The KLX02 waters seems to be the result of the former evolution pattern, i.e. mainly involving Modern Shallow, 60' Shallow and Old saline waters, although an input from the *Baltic Sea - Glacial meltwater* evolution may have caused some influence at depths shallower than 1000 m.

3.5.3 Mixing-mass balance calculations

A *Simple Mixing-Mass balance* model has been described by Laaksoharju (1990); Banwart et al.(1992); Smellie and Laaksoharju (1992). The main aim of the model is to differentiate in the groundwater between what is due to mixing and what is due to water/rock reactions. The starting point is that all groundwaters are to varying degrees a result of water/rock interactions and mixing according to:

Groundwater composition = Mixing + Water/rock interaction

In effect these two important processes are separated by the model. The mixing-mass balance model can describe how large the portions of a particular type of water are needed in order to explain the chemical composition of the observed water. The mixing ratios are then used to predict the water composition and the outcome of the predictions are compared to that observed. The model can only indicate a possible hydraulic connection and are always relative to the selected end-members.

The mixing-mass balance processes are inherently very complex and include fast/slow precipitation or dissolution reactions in combination with possible multi-end member mixing processes. The selection of a feasible end-member is therefore important for the outcome of the calculations. A standard method is to use univariate (e.g. x,y scatter plots) to identify the possible end-members. The obvious disadvantage is that the chemical variables can have different resolutions and magnitudes. There is also the known risk that information may be lost since similar changes or different scales in both the examined variables may mask or even bias the information. Also conservative tracers such as Cl may have more than one source i.e. Baltic sea and old saline groundwater. If Cl is used as an conservative tracer in such an instance, erroneous predictions will occur for mixing ratios and the mass balance calculations. The same applies for other so-called conservative tracers such as ^{18}O and ^{2}H which also may have a signature derived from mixtures of several sources. It is therefore necessary to use Principal Component Analysis (see section 3.5.2) to try to circumvent these disadvantages. The major components Cl, Ca, Na, Mg, K, SO_4 HCO_3 and the isotopes ^{2}H, ^{18}O and ^{3}H were used in the Principal Component Analysis. It is important to note that both conservative and non-conservative elements are used. This is possible since conservative or nonconservative behaviour in one or several of the variables can be separated by PCA. The identified end-members from the previous section (3.5.2) were therefore used (Figure 3-13).

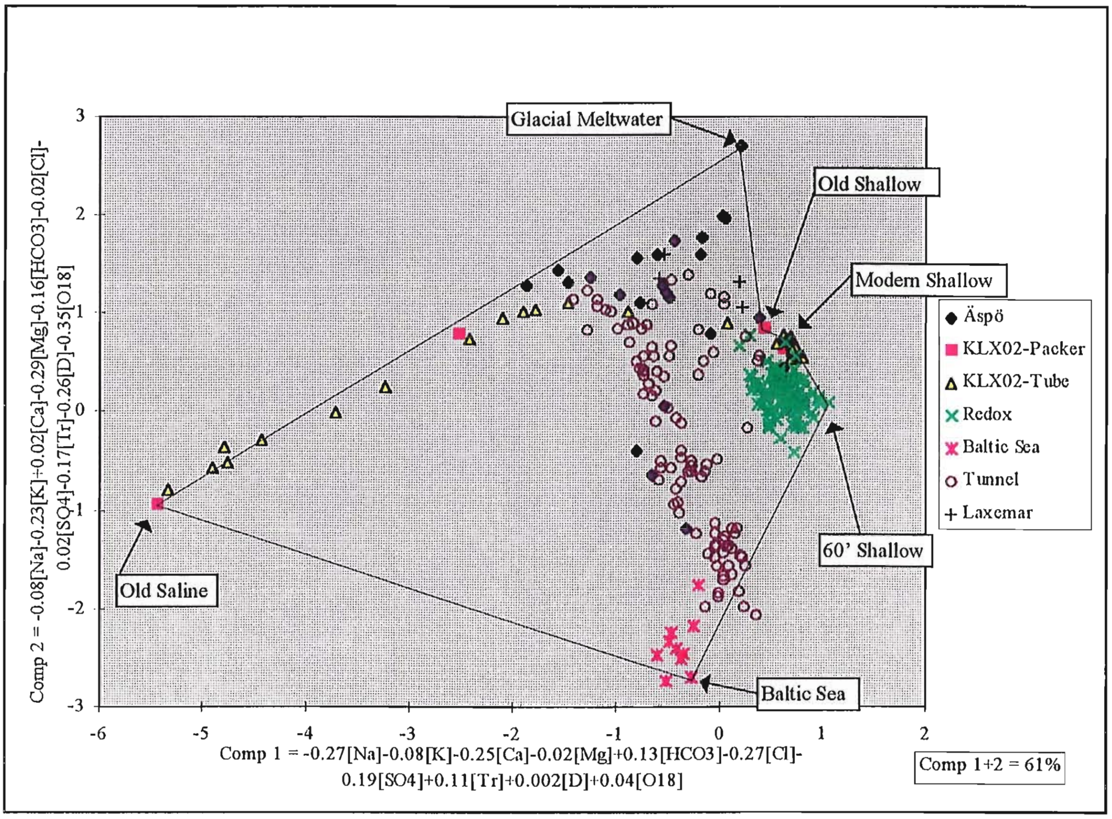


Figure 3-13: *Principal Component plot used for mixing calculations of the KLX02 waters. The position of the selected end-members are shown with black arrows. Between these six end-members a black line is drawn so a hexagon is formed. The observations within the hexagon can by definition be described by the selected end-members. The mixing ratios of any observed water in KLX02 can be calculated.*

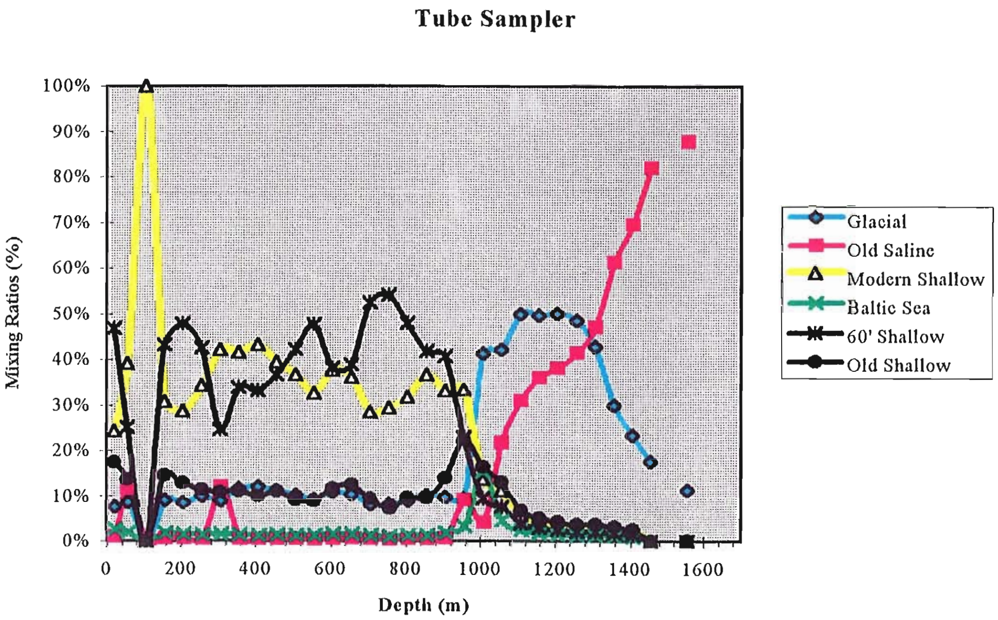
The six end-members in Figure 3-13 form a hexagon. The observations within the hexagon can by definition be described by the selected end-members. The co-ordinates for the observations are given by the first respective the second Principal Component (Comp 1 and Comp 2 in Figure 3-13). The distance from any observation to the six end-members can be calculated by using simple trigonometrical functions. The distance is equivalent with the mixing ratios of any observed water in the system. The calculated mixing ratios needed to explain the KLX02 water are shown in Table 3-8 and Figure 3-14a and b.

Table 3-8: The calculated mixing ratios for the KLX02 samples. The rounded mixing ratios add up to 100% in all the cases.

IDCODE	Sampler	SECUP (m)	SECLOW (m)	Average Depth (m)	Old Saline	Glacial melt	Baltic Sea	Old Shallow	60' Shallow	Modern Shallow	Sum
KLX02	SKB-packer	315	321.5	318	12%	7%	3%	15%	29%	35%	100%
KLX02	SKB-packer	335	340.8	338	11%	7%	3%	17%	27%	33%	100%
KLX02	SKB-packer	798	803.8	801	4%	14%	4%	39%	14%	25%	100%
KLX02	SKB-packer	1090	1096.2	1093	49%	46%	1%	2%	1%	2%	100%
KLX02	SKB-packer	1420	1705	1563	100%	0%	0%	0%	0%	0%	100%
KLX02	Tube sampler	9	31	20	1%	8%	3%	18%	47%	24%	100%
KLX02	Tube sampler	31	81	56	12%	9%	2%	14%	25%	39%	100%
KLX02	Tube sampler	81	131	106	0%	0%	0%	0%	0%	100%	100%
KLX02	Tube sampler	131	181	156	1%	9%	2%	15%	43%	31%	100%
KLX02	Tube sampler	181	231	206	1%	8%	2%	13%	48%	29%	100%
KLX02	Tube sampler	231	281	256	1%	10%	2%	11%	43%	34%	100%
KLX02	Tube sampler	281	331	306	12%	9%	2%	11%	25%	42%	100%
KLX02	Tube sampler	331	381	356	1%	12%	2%	11%	34%	41%	100%
KLX02	Tube sampler	381	431	406	0%	12%	1%	10%	33%	43%	100%
KLX02	Tube sampler	431	481	456	1%	11%	2%	11%	37%	39%	100%
KLX02	Tube sampler	481	531	506	0%	10%	1%	9%	42%	37%	100%
KLX02	Tube sampler	531	581	556	0%	9%	1%	9%	48%	33%	100%
KLX02	Tube sampler	581	631	606	1%	11%	2%	12%	38%	38%	100%
KLX02	Tube sampler	631	681	656	1%	10%	2%	12%	39%	36%	100%
KLX02	Tube sampler	681	731	706	0%	8%	1%	9%	52%	28%	100%
KLX02	Tube sampler	731	781	756	0%	8%	1%	7%	54%	29%	100%
KLX02	Tube sampler	781	831	806	0%	9%	1%	10%	48%	32%	100%
KLX02	Tube sampler	831	881	856	0%	10%	1%	10%	42%	37%	100%
KLX02	Tube sampler	881	931	906	1%	10%	2%	14%	41%	33%	100%
KLX02	Tube sampler	931	981	956	9%	9%	3%	22%	23%	33%	100%
KLX02	Tube sampler	981	1031	1006	4%	41%	15%	16%	9%	14%	100%
KLX02	Tube sampler	1031	1081	1056	22%	42%	5%	13%	8%	11%	100%
KLX02	Tube sampler	1081	1131	1106	31%	50%	2%	7%	4%	6%	100%
KLX02	Tube sampler	1131	1181	1156	36%	50%	2%	5%	3%	4%	100%
KLX02	Tube sampler	1181	1231	1206	38%	50%	2%	4%	3%	4%	100%
KLX02	Tube sampler	1231	1281	1256	41%	49%	1%	4%	2%	3%	100%
KLX02	Tube sampler	1281	1331	1306	47%	43%	1%	4%	2%	3%	100%
KLX02	Tube sampler	1331	1381	1356	61%	30%	1%	3%	2%	3%	100%
KLX02	Tube sampler	1381	1431	1406	70%	23%	1%	3%	2%	2%	100%
KLX02	Tube sampler	1431	1481	1456	82%	18%	0%	0%	0%	0%	100%
KLX02	Tube sampler	1531	1581	1556	88%	11%	0%	0%	0%	0%	100%

Abbreviations used in the table: IDCODE = Object identification code (in this report borehole name), SECUP = The upper limit of the borehole section, SECLOW = The lower limit of the borehole section.

A)



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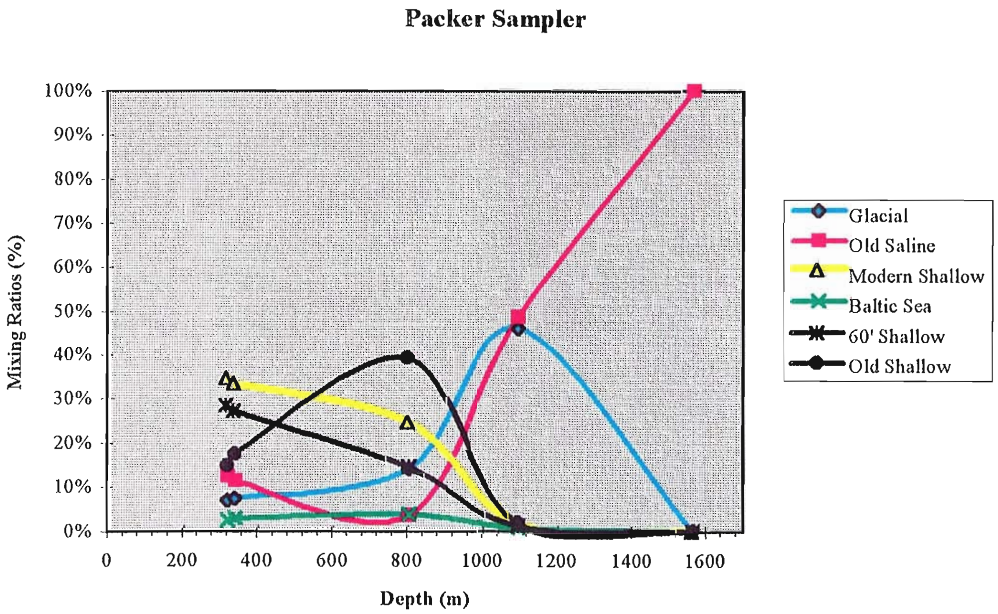
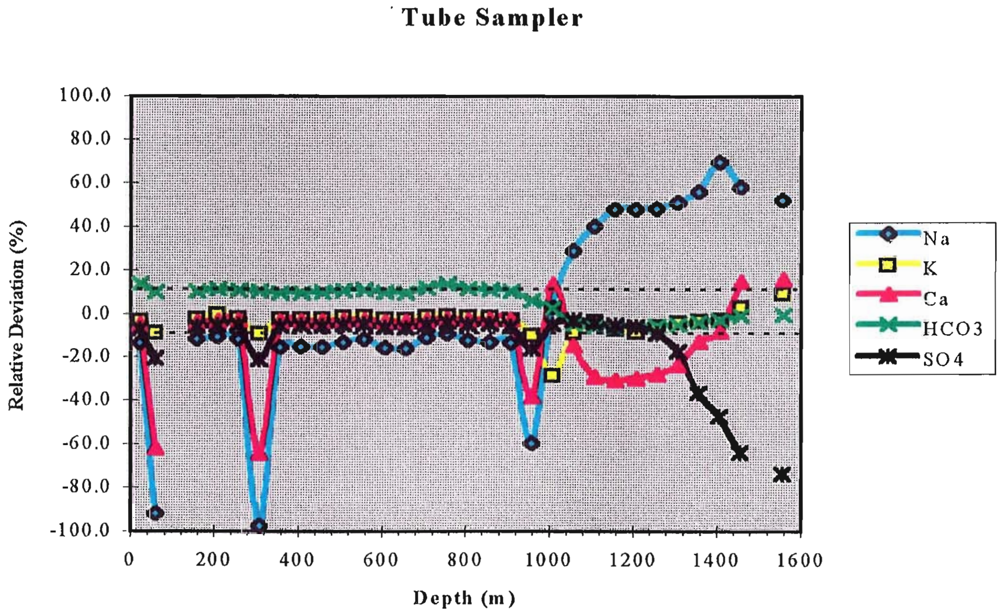


***Figure 3-14**: The mixing ratios versus depth of the KLX02 groundwaters. A) Tube sampler, B) SKB-packer sampler. The mixing ratios are calculated from the PC-analysis and results in 100% at respective depths. A mixing portion <10 % is regarded as uncertain.*

The above mixing ratio calculations describe the necessary portions of water needed from the end-members to achieve the measured water composition in Laxemar. In the samples from the Tube sampler a high portion of modern shallow water is seen in the upper part of the borehole (<100 m). At the 100-900 m depth shallow water from the 1960 (high tritium water) and modern shallow water dominates. At the 950 m depth an important portion (20%) of old shallow water occurs. At the deepest section of the borehole (1000-1600 m) glacial meltwater and old saline water dominates. The waters seem to form a time chronological sequence towards depth. In the samples extracted from the fractures a similar situation seems to prevail although the portion of old shallow water seems to be higher and the portion of shallow water from 1960 and modern shallow water is corresponding by lower.

When performing mass balance calculations the mixing ratios are used to predict new values for Na, Ca, HCO_3, SO_4 and K. The predicted values are then compared with the measured (Figure 3-15). Little or no deviation from the model predictions indicates that the concentration can be adequately explained by mixing; large deviations indicate sources or sinks for a particular element that are not accounted for by the mixing model. The reason for the deviation are mass balance reactions or influences from unknown end-members.

A)



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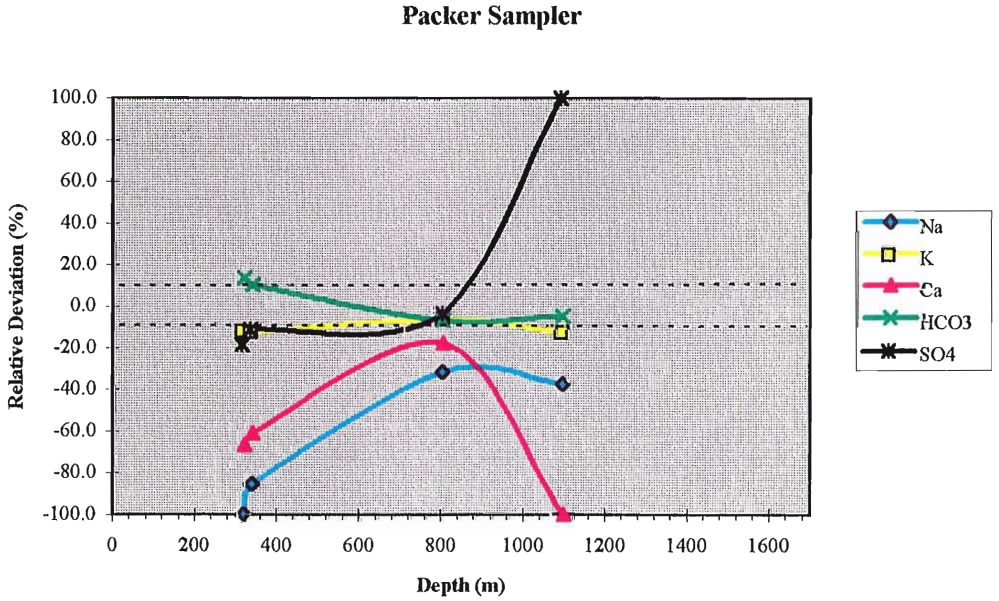

***Figure 3-15**: The results of the mass balance calculations show the deviation of the predicted water composition compared with observed KLX02 water. A high deviation from the observed indicates mass balance reactions; a lower deviation ± 10% within the dotted area may be explained by mixing. Loss of a particular constituent is indicated by a negative value and gain by a positive value. A) Tube sampler B) SKB-packer sampler.*

The mass balance calculations show that in the samples taken with the Tube sampler, a loss of Na and Ca occurs at 100 m, 350 m and 950 m depth. The loss may be explained by dilution from inflowing water. In the lower part >1000 m of the borehole Na is gained and Ca is lost which may indicate that ion exchange processes may be occurring. The SO_4 loss from the water at a depth >1300 m may indicate bacterial reduction. The gain of HCO_3 in the upper part of the borehole may indicate that oxidation of organic matter may be taking place. In the other part of the borehole regular mixing processes may explain most of the element behaviour (deviation <± 10%). In the samples taken with the SKB-packer sampler equipment a different picture evolves. Here a loss of Ca and a Na increase occurs in all observations; SO_4 gain is observed in the lower part of the borehole; the other constituents can be described by mixing. The reason for the different element behaviour between the open hole and fracture samples is not yet known, but open-hole mixing in the former caused by "natural" groundwater circulation or borehole activities prior to sampling is the most obvious possibility.

3.5.4 The high tritium values

Detectable tritium contents are present in all samples down to around 1000 m for the tube sampling method, and to the total length of the borehole using the SKB-packer sampling method. Mixing may be partly explained by natural recharge conditions (rapid influx via sub-vertical fracture zones) and partly explained by borehole activities such as drilling and hydrotesting during drilling. The long-term cleaning and test pumping (2.95 L/sec for 181 days) which was conducted during drilling and prior to hydrochemical sampling, may also have induced mixing. The borehole water sampled with the Tube sampler shortly after the end of the pumping period contained higher than 4.2 TU tritium contents (Figure 3-16), but only in the upper 1000 m of the borehole.

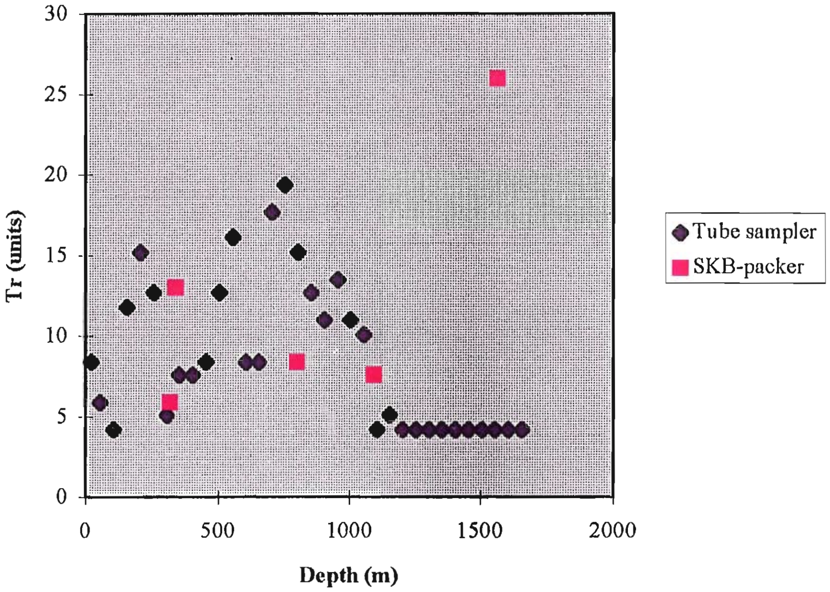

***Figure 3-16:** Tritium versus depth sampled in borehole KLX02.*

The high tritium content suggests either mixing with young, present-day near-surface waters (<35 yrs. old i.e. early 1960's), or, mixing of "old" tritium water (around 35 yrs. old) which is still present in formational groundwaters at these depths. Direct contamination from drilling water can be neglected as uranine is consistently less than 1%. The presence of "old" tritium water is also suggested by a tritium content of 26 TU at the 1420 m level; this is too high for present-day input (max. 22 TU). The mixing calculations support the idea that tritium is correlated with water from 1960 and less with modern shallow water or old saline water (Figure 3-17a, b and c). The conclusion from the mixing calculations are that borehole waters contain both "young" and "old" tritium components, but the water from 1960's has influenced more the tritium content during sampling. It is important to remember that precipitation 1960 could contain up to 3000 tritium units. The radioactive half-life of tritium is 12.43 years. Theoretically a groundwater sampled today could contain 833 TU (sample from Taavinunnanen (KTA:654-700 m = 176 TU)). A few percent of this kind of water mixed with deep water could well explain the high tritium values measured in Laxemar. The mixing calculations indicate that the high tritium content in the 1090-1096.2 m section are due to contamination by 1% shallow water from 1960 and 2% of modern shallow water. These mixing ratios predict a tritium content of 8.8 TU (0.01 * 833 TU + 0.02 * 22 TU = 8.8 TU) in the borehole section. The predicted value is in good agreement with measured 7.6 TU. Alternative explanations such as in-situ production of tritium have been considered but this has been judged unlikely because of an absence of uranium mineralisation in the area. This phenomenon will, however, be further investigated.

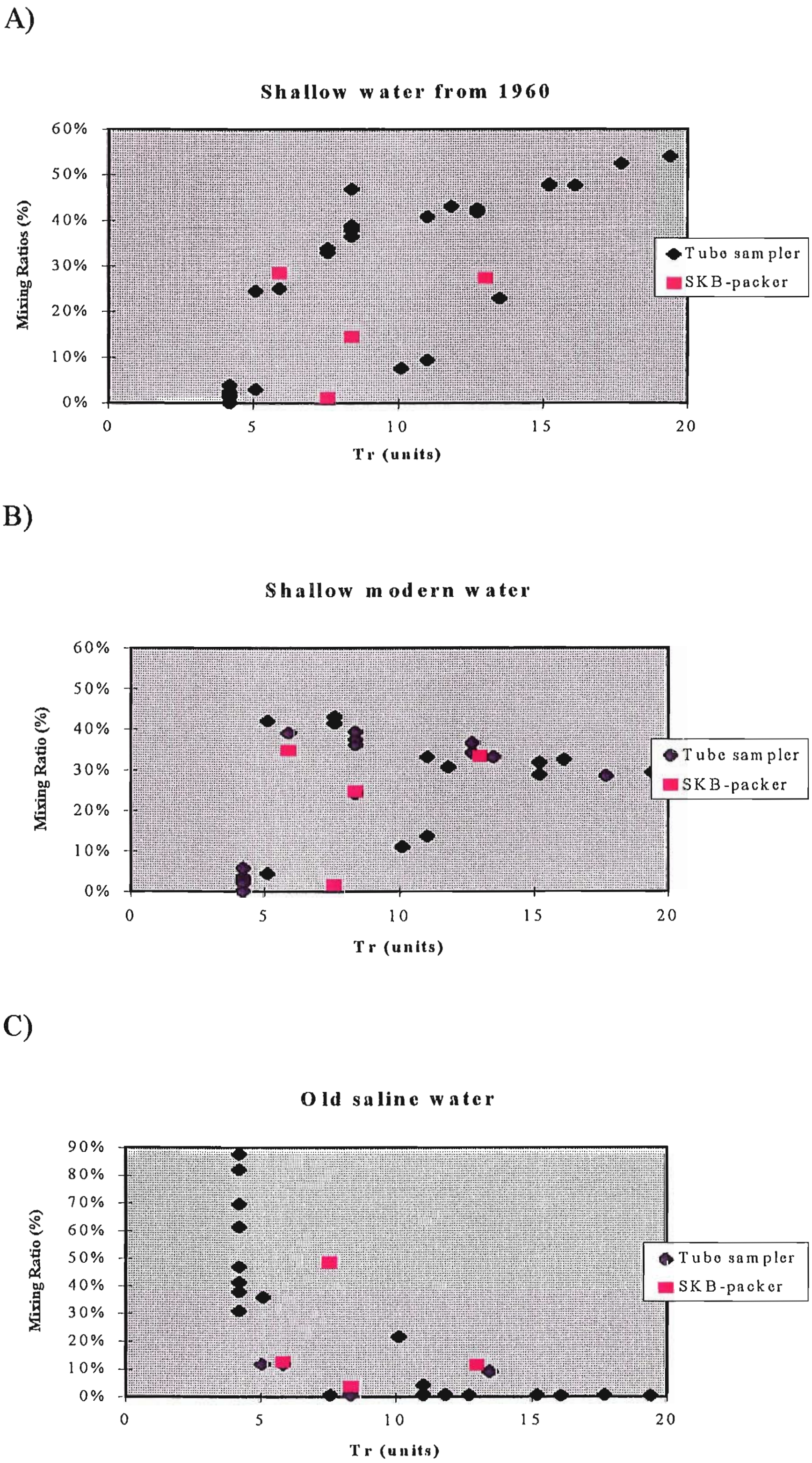

Figure 3-17: *a) Water portions of shallow water from the 1960's in KLX02 versus measured tritium content in groundwater. b) Water portions of modern shallow water in KLX02 versus measured tritium content in the groundwater. c) Water portions of old saline water in KLX02 versus measured tritium content in the groundwater.*

3.6 Summary and discussion

The groundwaters from borehole KLX02 at Laxemar show two distinct groupings, shallow to intermediate brackish waters and deep brines; the former are meteoric in origin and the latter are typical basement brines similar to those described from the Canadian Shield. The transition between both types is sharp, at least over a distance of 300 m (800-1100 m depth). No reliable structural model exists, but detailed core mapping of KLX02 shows two areas of low fracture frequency; down to 700-750 m and from 1100-1500 m. Significantly, the latter corresponds to the occurrence of the high saline groundwaters; this is supported by the flow meter measurements which show very low hydraulic conductivity for this deep section (Figure 2-1). The former, down to 700-750 m, show higher hydraulic conductivities; these are characterised by brackish groundwaters and there is evidence of mixing of different end-members. From 750 to 1100 m there is an increase in fracture frequency but a decrease in overall hydraulic conductivity. Within this interval there also occurs several important fractures, especially at 800-900 m and 1100 m which show strong reflections in the electrical conductivity measurements. Downhole radar measurements show that some of the major fractures intersect KLX02 at moderate angles (40-45°), whilst other fractures are known to be sub-vertical in orientation; there is a strong suggestion that some of these fractures extend to near the bedrock surface.

The working hypothesis at the moment is that the upper 800 m of bedrock at Laxemar lies within a groundwater recharge area; the sub-vertical to moderate angled fracture zones facilitate groundwater circulation and mixing to considerable depths, at least to 800 m, thus accounting for some of the low saline brackish groundwaters in these conducting fracture zones. Mixing of different groundwater end-members to these depths is illustrated by the major ion and isotope chemistry, and supported by modelling conclusions. Below 1100 m the system is hydraulically and geochemically "closed" such that highly saline groundwaters exist in a near-stagnant environment. These Ca-Cl dominated brines represent deep regional groundwaters where long residence times and water-rock interactions have played a dominant role in determining their composition.

Some artificially induced mixing of groundwaters may also have occurred in the upper 1000 m of the borehole due to earlier borehole activities; there is an absence of flushing water contamination, i.e. all sampled waters contain less than 1% uranine. Three major activities may have influenced the groundwater system: 1) the hydraulic testing during drilling, 2) the long-term maintenance pumping prior to groundwater sampling, and 3) open-hole effects and mixing due to borehole activities.

Open-hole effects are difficult to quantify because of insufficient hydraulic data (e.g. water budget calculations) from each of the hydraulically conducting zones sampled.

The influence of these borehole activities are seen in the tritium data which records significant tritium down to 1000 m, and even to 1420 m in samples collected by the SKB-packer sampling method. Recharge tritium values are around 22 TU such that mixing and dilution can account for the present distribution of values. However, at one level (1420 m) the presence of 26 TU (i.e. in excess of present-day recharge at 22 TU) suggests that one of the mixing end-members may be "old" tritium waters (up to 35 yrs). Mixing modelling showed that water from 1960 is the main source for tritium. This water may have been drawn into the borehole at various levels but mostly from above 700-1000 m depth during the hydraulic testing and the long-term maintenance pumping. Tritium levels might have been higher but mixing and dilution have probably reduced the content. Alternative explanations such as in-situ production of tritium have been considered possible, but because of an absence of uranium mineralisation in the area. This explanation is regarded as less probable. In general, the tritium data (supported by the mixing models) illustrate the complex mixing of the sampled borehole waters. Because the main causes are believed to be artificially induced, the representativeness of the lower groundwater samples may be questioned. However, the high tritium values in the 1090-1096.8 m section are due to contamination of 1% shallow water from 1960 and 2% of modern shallow water. This is not believed to have affected the representativeness of the water dramatically. The major results from the KLX02 investigation are shown in Figure 3-18.

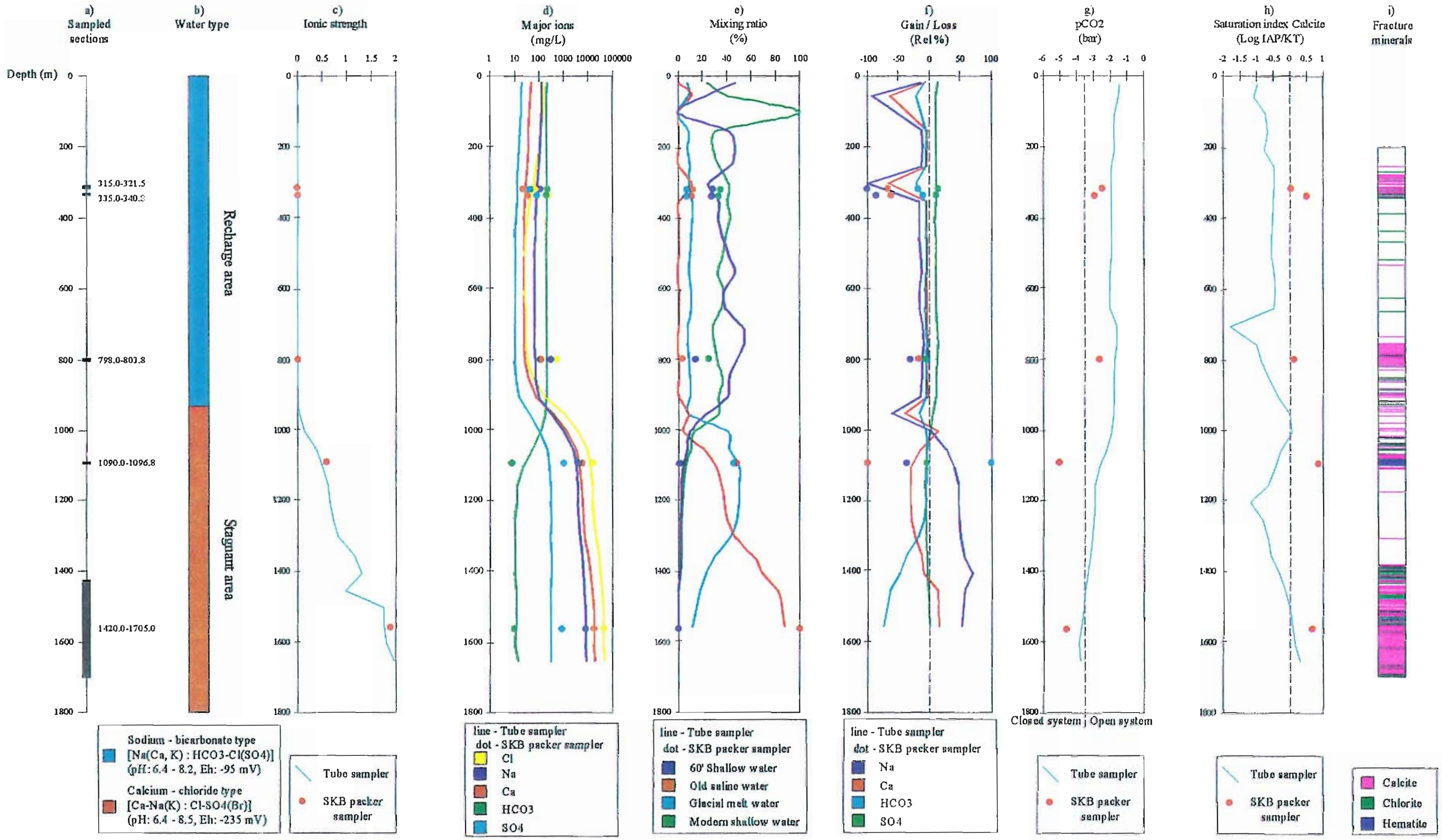

Figure 3-18. *Overview and summary of the major results from the KLX02 investigation; a) the sampled sections using the SKB-packer sampler; the whole borehole length was sampled using the Tube sampler; b) the two major water types; c) the ionic strength of the water; d) the distribution of the major ions; e) the calculated mixing ratios; f) the mass balance calculations showing the gains/losses of major components due to reactions; g) calculated partial pressure of carbon-dioxide using PHREEQE (Parkhurst et al., 1989); the lower part of the borehole represent a closed system (the pH values for the tube samples are uncertain and hence the calculations are questionable); h) saturation indices for calcite show a close or super-saturation for the SKB-packer samples (the pH values for the tube samples are uncertain and hence the calculations are questionable) this is in good agreement with the most common fracture mineral in KLX02 calcite; i) the major fracture minerals.*

4. Conclusions and future implications to site specific studies

The main purpose of a hydrogeochemical site characterisation for repository containment is to establish the chemistry of the different groundwater types, their origin, their evolution, the dominant reactions and reactive processes within the host bedrock that determine the chemical and isotopic character of the groundwaters, the degrees of groundwater mixing and, ultimately, to trace the groundwater flow patterns. Only when this has been achieved is it possible to predict the behaviour of a radioactive repository system in the event of potential changes in groundwater composition, for example, due to drastic climatic changes (i.e. glacial scenario), and the far-field chemical controls acting on radionuclide mobility and transport in the event of radionuclide leakage and dispersion from a breached waste package.

In the Fennoscandian Shield environment of Sweden, where groundwater flow through crystalline bedrock is controlled by complex systems of fractures, experience has shown that every fracture system is unique and, depending on its hydraulic properties, may reflect, in terms of contamination, a history of borehole activities prior to sampling. This was clearly illustrated in the early SKB site investigations (Smellie et al., 1985, 1987) and later at Äspö (Smellie and Laaksoharju, 1992). Drilling, borehole clearance, geophysical logging, hydraulic testing (injection and interference) and eventually groundwater sampling can all contribute to reduced groundwater quality and a lack of representativeness for the bedrock level under investigation (Laaksoharju et al., 1993; Smellie et al., 1994).

The deep borehole at Laxemar was planned as a test-case for future site-specific investigations with the central aim of efficiently and quantitatively characterising the groundwater chemistry. Earlier SKB site-specific investigations did not include deep boreholes intended mainly for hydrogeochemical studies. In most cases these earlier programmes involved up to 15 cored boreholes (to maximum depths of 700-800 m) for complete site characterisation. Because of rigid time schedules and lack of experience in recognising the sensitivity of groundwaters to borehole activities, the hydrogeochemical programmes normally constituted the final stages of the investigations, with the result that many of the boreholes were contaminated to varying degrees prior to sampling.

Of considerable importance is the pre-monitoring stage, i.e. the initial location of the boreholes, the drilling techniques employed, whether sampling should be carried out both during and subsequent to drilling, and borehole activities conducted prior to the main sampling programme (e.g. hydraulic testing; geophysical logging). These topics have been fully presented and discussed by Laaksoharju et al. (1993) and Smellie et al. (1994). Taken collectively, it was strongly felt that the integrity of hydrogeochemical studies would benefit considerably from: a) first locating a deep borehole (1000 m) solely to establish the reference hydrogeochemistry (reference source term), b) establishing a routine protocol of pre-monitoring, monitoring, sampling and analysis for the hydrogeochemical borehole, and c) establishing a routine protocol of pre-monitoring, monitoring, sampling and analysis for all subsequent boreholes.

Many of these criteria were included in the planning of the Laxemar deep borehole programme. The borehole was placed strategically on the mainland, adjacent to the Äspö Hard Rock Laboratory site, to investigate the origin and chemistry of deep basement groundwaters which until now have been largely neglected in Sweden. These data, together with other regional studies (e.g. Klipperås), would subsequently be used in establishing deep regional trends around the Äspö area. This in turn would allow the groundwater studies at Äspö to be interpreted in a more regional context.

The successes and drawbacks of the Laxemar programme can be summarised in the following conclusions:

- Drilling - largely successful apart from the leakage between the outer casing and borehole rim at around 200 m. This may have had some repercussions on the pump-tests carried out during and after drilling. During this pumping low Cl-contents were detected a great depths which indicates significant inflow of shallow groundwater.

- Pumping - periodic maintenance pumping was carried out over a considerable period of time with little monitoring of groundwater chemistry to record any change in chemical parameters. This pumping may have influenced groundwater mixing in the borehole.

- Detailed chemical characterisation during drilling - due to a strict time schedule this was not possible. This was unfortunate as this procedure may have located more precisely the transition from brackish to highly saline groundwater types.

- Borehole activities - activities carried out prior to hydrochemical sampling included calliper measurements, geophysical logging, radar and flow-meter measurements. All these methods can cause perturbation to the borehole water. Earlier studies recommended that only those methods essential to locate potentially conducting horizons for hydrochemical sampling should be carried out prior to sampling, i.e. calliper, radar and flow-meter. The remainder should be carried out after sampling is complete to minimise groundwater perturbation.

- Sampling locations - these were based on drillcore mapping, radar data and flow-meter measurements. The lack of hydrotest data required extra time when lowering and uplifting the SKB-packer sampler when testing and locating water conducting fractures in the borehole. However, this perturbation is of less importance when compared to disturbances from the regular hydrotests. The chosen locations were largely successful, although in retrospect at least one more strategic location within the 300-800 m section should have been sampled. Time constraints prohibited this.

- <u>Tube sampling</u> - this was successfully carried out and gave valuable information. The main reservation is that samples represent open-hole conditions which require quantitative borehole hydraulic data (e.g. hydraulic head; water budget calculations etc.) to interpret. These hydraulic data are not available. The pH measurements were conducted up to four days after sampling which made them unreliable.

- <u>SKB-packer sampling</u> - this was largely successful with some reservation at the 798-803.8 m level where packer installation difficulties were encountered. The total time spent at the borehole was 129 days; the effective sampling time was 86 days i.e. 67% of the total time was effective sampling. The rest of the time was spent dealing with technical problems. In general 3-5 days more per section could have improved the representativeness of some of the samples. Field personal estimated that a total of 25 days more (5 days flexibility per section) would significantly improve the working conditions and the quality (Nederfeldt pers. comm).

- <u>Pre-monitoring</u> - monitoring of pH, Eh, cond. and temp. in the groundwaters proved to be very useful in determining when sampling should commence and which sample should be chosen as most representative. It also underlined the many difficulties (mechanical and instrumental) which can occur during normal sampling procedures. Because of the time restrictions these pre-monitoring periods were too short; greater flexibility in future is recommended.

- <u>Sample representativeness</u> - all samples show significant levels of tritium. This has been explained by: a) the mixing of "old" tritium waters (up to 30 yrs. old) in various proportions with tritium-free formation waters, and b) mixing of "young" tritium waters (less than 30 yrs.) with tritium-free formation waters. Mixing calculations showed that the first process explains most of the tritium values. Mixing of such waters to depths of 900 m and even down to 1420 m may be partly normal (active recharge), but mixing processes are believed to have been influenced mainly by drilling, pumping and borehole activities. Drilling water is consistently less than 1% uranine and is therefore not a source of contamination. In conclusion, the high tritium values in the lower sections (e.g. 1090-1096.2 m) are due to contamination of 1% shallow water from the 1960's and 2% of modern shallow water. This may to some degree have affected the representativeness of the deeper waters.

- Groundwater chemistry - two distinct groundwater types can be identified: shallow to intermediate brackish type of meteoric origin (0-1000 m), and a deep basement brine type (1000-1700 m), similar to those reported from the Canadian Shield. Mixing between both types is evident; this has probably been influenced by borehole activities. Laxemar has been compared with the Äspö site and shows that the regional brines represent the more evolved end-member of the deepest waters sampled at Äspö. This has been clearly illustrated by different modelling approaches.
- Recommendations - the Laxemar experience has fulfilled many of the earlier recommendations to improve groundwater sampling for hydrogeochemical purposes. Further improvements need to be further implemented: a) sampling during drilling, b) no major pumping until hydrochemical sampling is complete, c) much of the geophysical logging should be carried out after sampling has been completed; only calliper, radar and flow-meter measurements are required, and d) more time (3-5 days) for pre sampling monitoring of pH, Eh, cond. and temp. to ensure representative sampling conditions. Further improvements in cleaning the water tube should be further investigated. Reporting of field activities should be conducted shortly after sampling so that valuable knowledge from field personnel is not lost.

5. Acknowledgments

The authors want to thank Peter Wikberg, SKB who initiated the investigation and provided valuable comments during preparation of the manuscript. Additional comments and suggestions from Fred Karlsson, SKB, and Lars O. Ericsson, SKB are greatly acknowledged. Erik Thurner, SKB, provided the necessary background information for the activities carried out in the borehole. Karl-Göran Nederfeldt, ÅF-IPA, performed the practical field investigations and contributed with his extensive field knowledge.

6. References

Almén K-E, Andersson J-E, Carlsson L, Hansson K, Larsson N-Å, 1986. Hydraulic testing in crystalline rock. A comparative study of single-hole test methods. SKB Technical Report TR 86-27.

Axelsen K, Wikberg P, Andersson L, Nederfelt K-G, Lund J, Sjöström T, Andersson O, 1986. Equipment for deep groundwater characterisation: calibration and test run in Fjällveden. SKB Status Report AR 86-14.

Back W, 1966. Hydrochemical facies and ground-water flow patterns in northern part of Atlantic Costal Plain. U.S. Geol. Surv. Prof. Paper 498-A. 42 pp.

Banwart S, Laaksoharju M, Nilsson A-C, Tullborg E-L, Wallin B, 1992. The large-scale redox experiment: Initial characterization of the fracture zone. SKB Progress Report PR 25-92-04.

Carlsten S, 1994. Drilling KLX02-Phase II Lilla Laxemar, Oskarshamn. Correlation of radar reflectors between boreholes KLX01 and KLX02. SKB Progress Report AR 94-28.

Chatfield C and Collins A J, 1989. Introduction to multivariate analysis. Chapman and Hall. 216 p.

Davis S N and De Wiest R J M, 1967. Hydrogeology, 2d Ed., John Wiley & Sons, New York, 436 p.

Follin S, 1993. Äspö Hard Rock Laboratory. Evaluation of hydraulic tests conducted during the completion of borehole KLX02. Lund University Report.

Frape S K and Fritz P, 1987. Geochemical trends for groundwaters from the Canadian Shield. Geol. Assoc. Canada, Spec. Paper, 33.

Gåal G and Gorbatschev R, 1987. An outline of the Pre-cambrian evolution of the Baltic Shield, Precambrian Research 35, 15-52,1987.

Grenthe I, Stumm W, Laaksoharju M, Nilsson A-C, Wikberg P, 1992. Redox potentials and redox reactions in deep groundwater systems, Chemical Geology, 98, 131 150, 1992.

Johansson Å, 1988. The age and geotectonic setting of the Småland Värmland granite poryphry belt, Geologiska Föreningens i Stockholm Förhandlingar, 110, 105 110, 1988.

Laaksoharju M and Nilsson A-C, 1989. Models of groundwater composition and of hydraulic conditions based on chemometrical and chemical analyses of deep groundwater at Äspö and Laxemar. SKB Progress Report PR 25-89-04.

Laaksoharju M, 1990. Measured and predicted groundwater chemistry at Äspö. Royal Institute of Technology, Stockholm. SKB Progress Report PR 25-90-13.

Laaksoharju M, Smellie J, Ruotsalainen P, Snellman M, 1993. An approach to quality classification of deep groundwaters in Sweden and Finland. SKB Technical Report TR 93-27.

Laurent S, Magnusson S, Nilsson A-C, 1992. Description of groundwater chemical data in the SKB database GEOTAB prior to 1990. SKB Technical Report TR 92-10.

Morgan C O and Winner M D Jr, 1962. Hydrochemical facies in the 400 foot and 600 foot sands of the Baton Rouge Area, Louisiana. U. S. Geol. Surv. Prof. Paper 450-B, pp. B 120-121.

Nordstrom D K, 1989. Application of a cation exchange mass balance model to the interpretation of saline groundwater chemistry evolved from Holocene seawater entrapped in rapakivi granite at Hästholmen, Finland. Proceedings of the 6th International Symposium on Water-rock Interaction, Malvern 1989.

Nurmi P A and Kukkonen I T, 1986. A new technique for sampling water and gas from deep drill holes. Canadian Journal of Eart Sciences. Volume 23, Number 9, 1986 (pages 1450-1454).

Parkhurst D L, Thorstenson D C, Plummer L N, 1980. PREEQE - A computer program for geochemical calculations: U.S. Geological Survey Water Resources Investigation Report 80-96, 210 p.

Piper A M, 1953. A graphic procedure in the geochemical interpretation of the water analyses, U.S. Geological Survey, Water Res. Div. Ground Water Notes, Geochemistry. no. 12, 14 pp.

Smellie J, Larsson N-Å, Wikberg P Carlsson L, 1985. Hydrochemical investigations in crystalline bedrock in relation to existing hydraulic conditions. Experience from the SKB test-sites in Sweden. SKB Technical Report TR 85-11.

Smellie J, Larsson N-Å, Wikberg P, Puigdomenech I, Tullborg E-L, 1987. Hydrochemical investigations in crystalline bedrock in relation to existing hydraulic conditions: Kråkemåla test-site, Småland, Southern Sweden. SKB Technical Report TR 87-21.

SKB MD 430-434. SKB manuals and method descriptions.

Smellie J and Laaksoharju M, 1992. The Äspö hard rock laboratory: final evaluation of the hydrogeochemical pre investigations in relation to existing geologic and hydraulic conditions. SKB Technical Report TR 92-31.

Smellie J, Laaksoharju M, Snellman M, Ruotsalainen P, Wikberg P, 1994. Groundwater quality and sampling strategy based on experience derived from the Finnish and the Swedish radioactive waste disposal programmes (in prep.).

Smellie J, Laaksoharju M, Wikberg P, 1995. Äspö, S.E. Sweden: A natural groundwater flow model derived from hydrogeochemical observations. Jr. Hydrol., (In press).

Wikberg P, 1987. The chemistry of deep groundwaters in crystalline rocks. Thesis of Inorganic Chemistry, KTH, S-10044 Stockholm, Sweden.

Wikström L and Björklund A, 1994. Trace elements in waters of low-conductivity rocks in the Äspö Hard Rock Laboratory. SKB Progress Report PR 25-94-28.

Wold S, 1987. Principal component analyses. Chemometric and Intelligent Laboratory Systems, 2, 35-37.

7. Appendix 1: Tube sampler results as matrix scatter plots

Chemical analyses of samples collected using the Tube sampler method, shown as matrix scatter plots with histograms. The values are presented numerically in Table 3-3. Abbreviations used in the figure: SO4S = SO_4-S (Sulphur by ICP-AES), H2 = deuterium, H3 = tritium, O18 = oxygen-18.

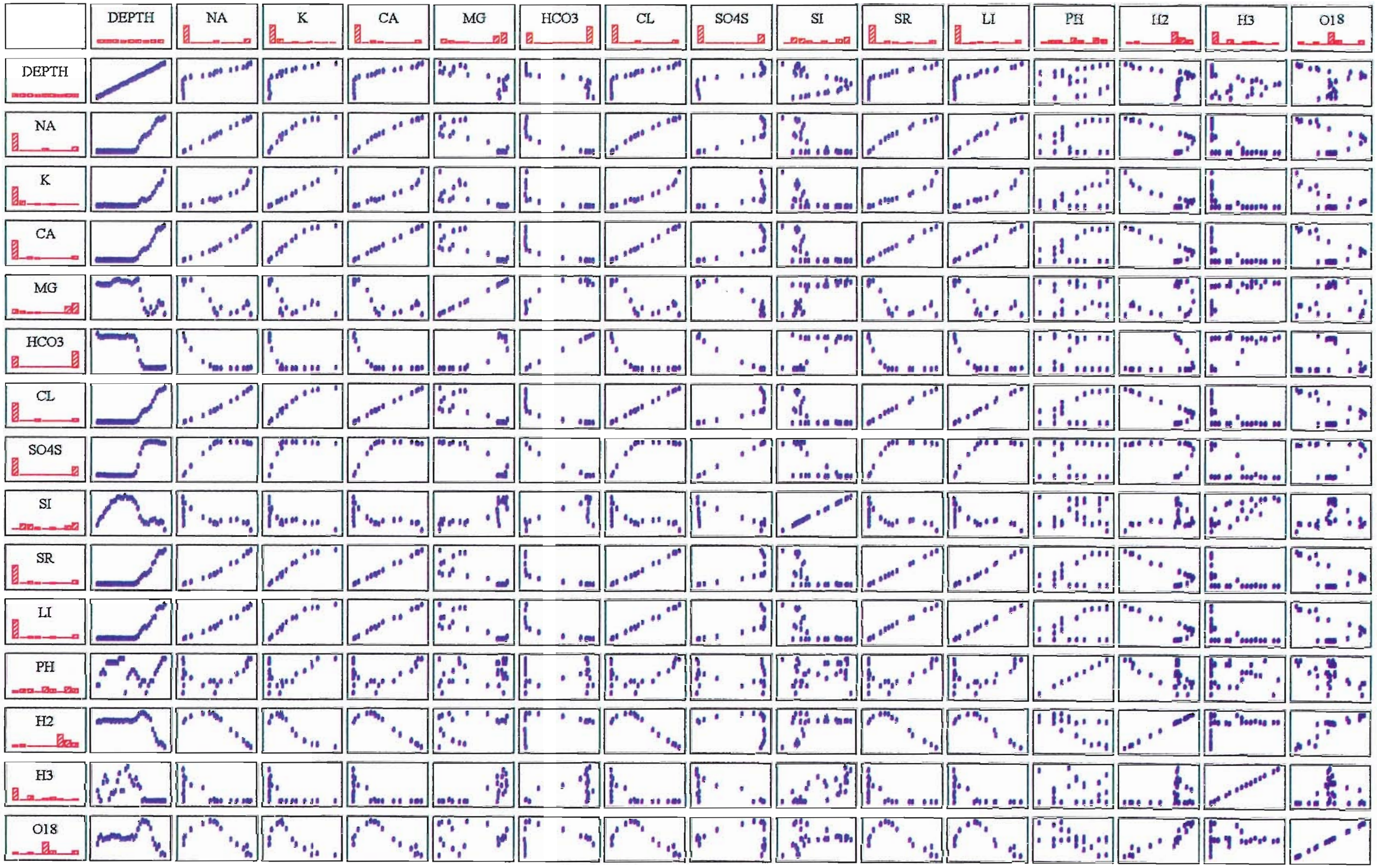

Figure 7-1: Chemical analyses of samples collected using the Tube sampler shown as matrix scatter plots with histograms.

8. Appendix 2: SKB-packer sampler results as matrix scatter plots

Chemical analyses of samples collected using the SKB-packer sampler method, shown as matrix scatter plots with histograms. The values are presented numerically in Table 3-4. Abbreviations used in the figure: SO4S = SO_4-S (Sulphur by ICP-AES), PO4P = PO_4-P, NO2N = NO_2-N, NH4N = NH_4-N, H2 = deuterium, H3 = tritium, O18 = oxygen-18, COND = Manual measurement of electrical conductivity in the laboratory, WFLOW = Water flow rate, DRILLW = Drilling water residue.

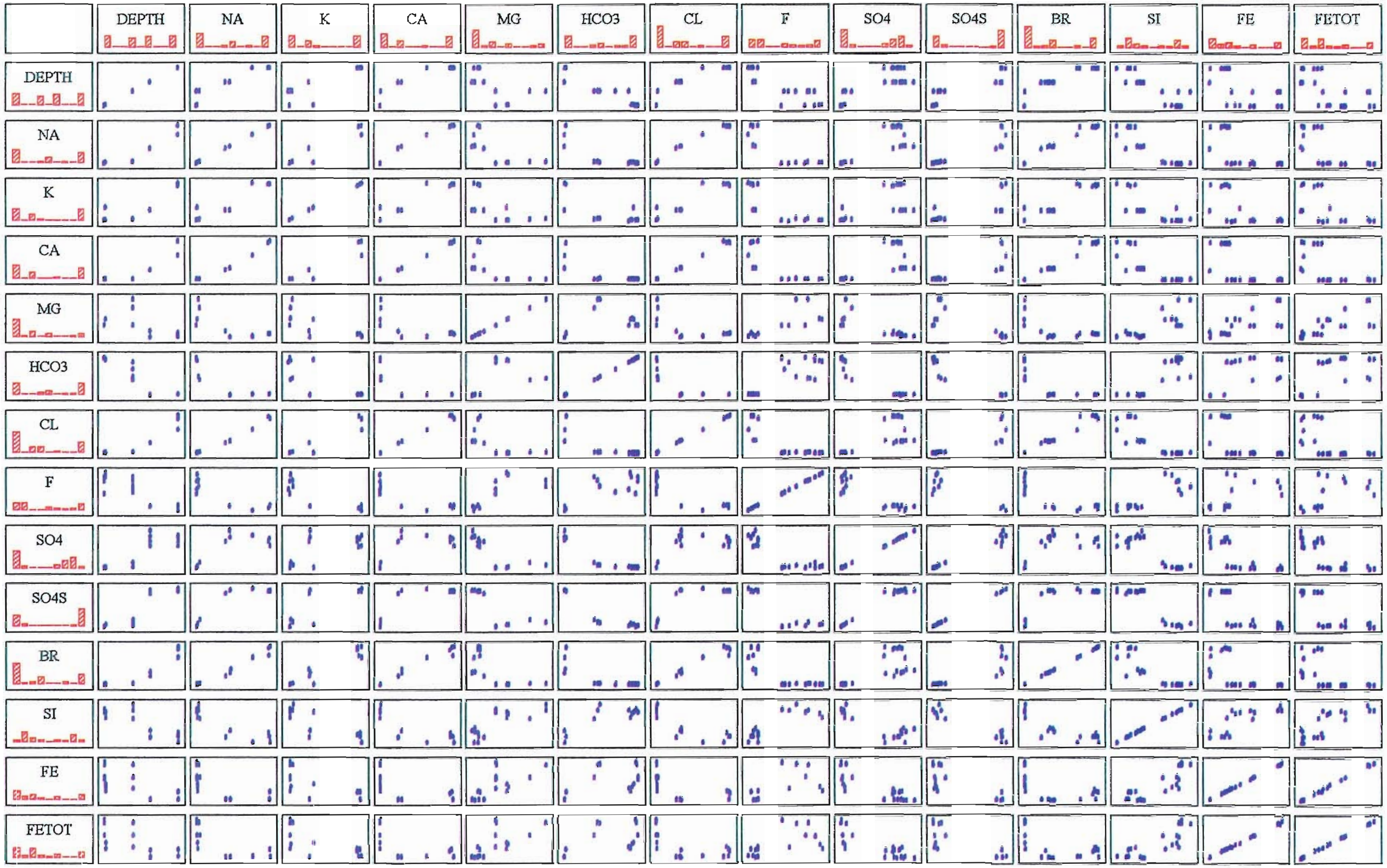

Figure 8-1: *Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

Figure 8-1: Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.

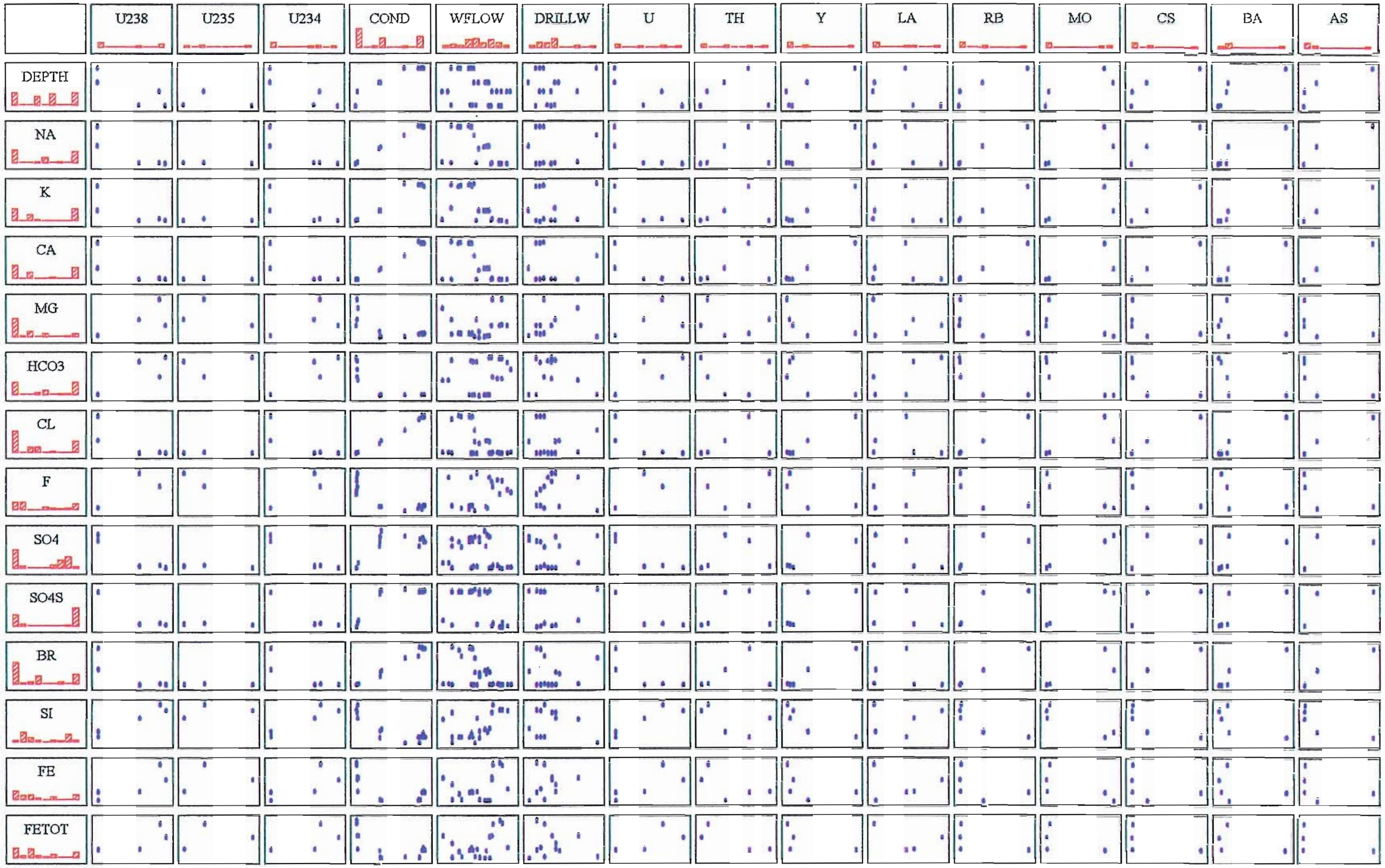

Figure 8-1: *Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

Figure 8-1: *Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

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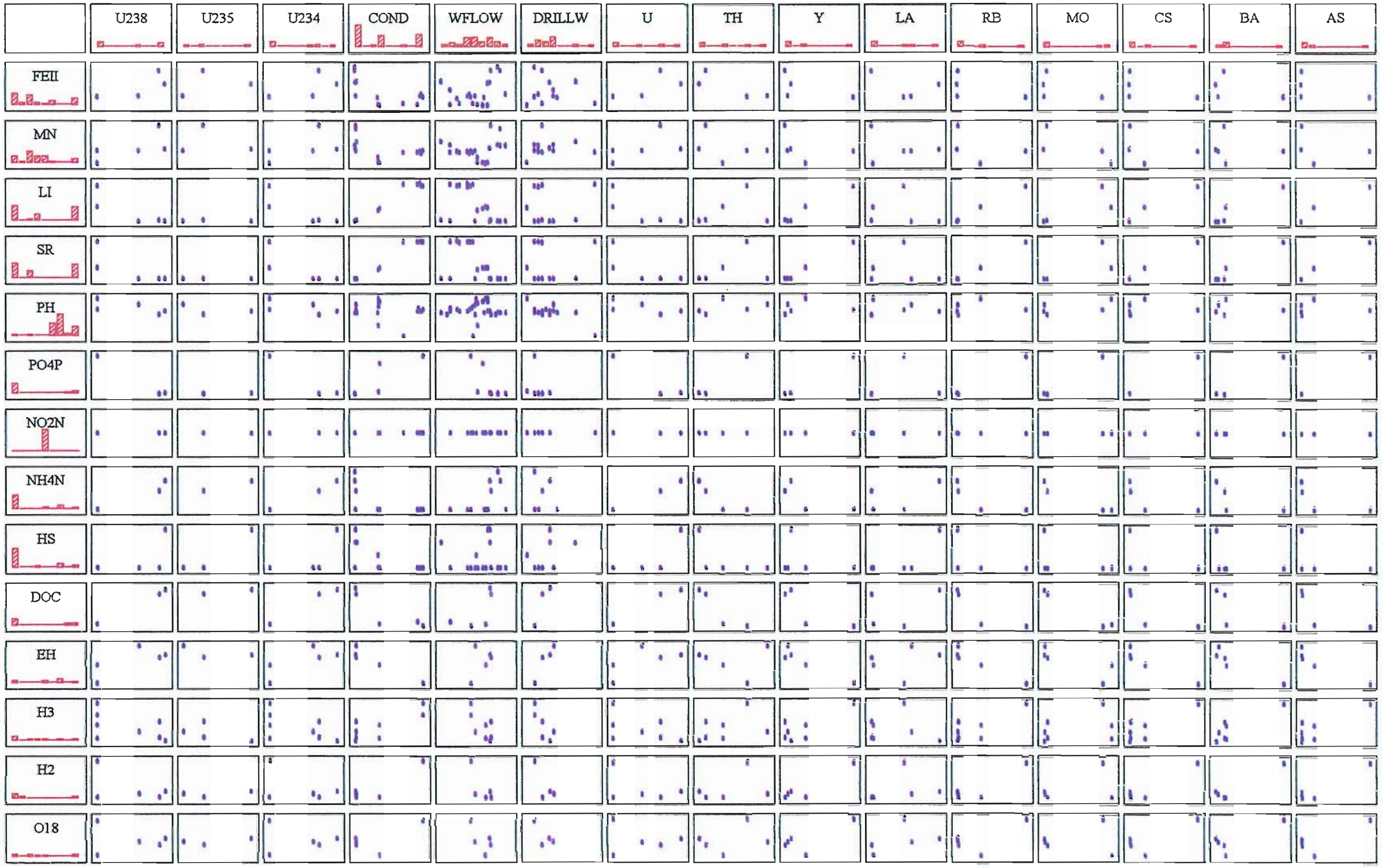

***Figure 8-1:** Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

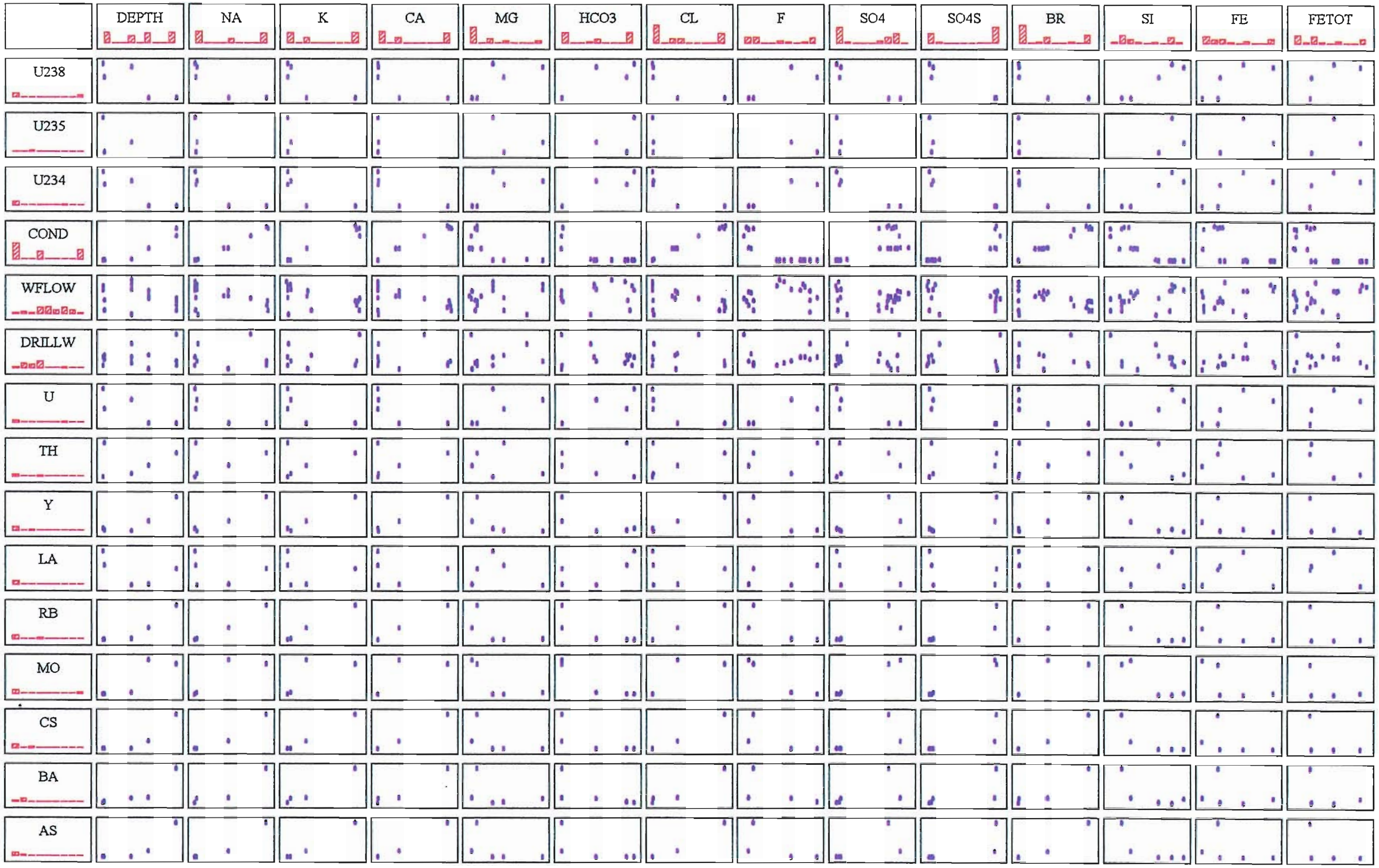

Figure 8-1: *Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

Figure 8-1: *Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.*

Figure 8-1: Continued. Chemical analyses of samples collected using the SKB-packer sampler shown as matrix scatter plots with histograms.

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Maria Malmström[1], Steven Banwart[1], Lara Duro[2], Paul Wersin[3], Jordi Bruno[3]

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[2] Universidad Politécnica de Cataluña, Departmento de Inginería Química, Barcelona, Spain

[3] MBT Tecnología Ambiental, Cerdanyola, Spain

January 1995

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Lars Werme, Joachim Eriksson

Swedish Nuclear Fuel and Waste Management Co, Stockholm, Sweden

March 1995

TR 95-03

Prestudy of final disposal of long-lived low and intermediate level waste

Marie Wiborgh (ed.)

Kemakta Konsult AB, Stockholm, Sweden

January 1995

TR 95-04

Spent nuclear fuel corrosion: The application of ICP-MS to direct actinide analysis

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March 1995