

Oskarshamn site investigation

**Borehole KLX17A
Characterisation of pore water**

**Part 1 Methodology
and analytical data**

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September 2007

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Keywords: Pore water extraction, Drillcore material, Chemical and stable isotope (^2H and ^{18}O) analysis, groundwater ^{36}Cl data.

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Abstract

In borehole KLX17A samples for pore water investigations were successfully collected along the total length of the borehole and along a profile from a water-conducting deformation zone into the deeper, intact bedrock matrix. During the Holocene various major periods with different groundwater chemistry (e.g. Glacial, Littorina Sea, Baltic Sea) characterised the fracture groundwaters in the Laxemar subarea to varying depths and extent. This present investigation aimed to characterise pore waters along the borehole and also the interaction between stagnant pore water and circulating fracture groundwater obtained from a continuously-sampled profile from a hydraulically active deformation zone into the surrounding intact rock matrix. These data can be used to try and resolve the palaeohydrochemical records archived in the pore water. The methodology to extract and analyse the pore water is outlined and the raw analytical data are tabulated.

Pore water that resides in the connected pore space in the matrix of crystalline rocks interacts continuously with groundwater circulating in the fractures which demarcate the blocks of low-permeability in the bedrock mass. The extent of such interaction depends on the hydraulic properties of the rock matrix and the water-conducting fracture(s), the chemical gradient established between pore water and fracture groundwater, and the time of groundwater circulation in the fracture. As part of the Oskarshamn hydrogeochemical site investigation programme, pore water investigations in borehole KLX17A aimed to characterise pore waters along the borehole and also the interaction between stagnant pore water and circulating fracture groundwater obtained from a continuously sampled profile from a hydraulically active deformation zone into the surrounding rock matrix.

Included as Appendix A to this report are groundwaters sampled from the water-conducting deformation zone which marked the starting point of the sampled pore water profile. Included as Appendix B are ^{36}Cl age data from selected groundwater types that characterise the subareas within the Oskarshamn site investigation area. This information is important as it provides support to the site description model both hydrochemically and from a palaeohydrogeochemical viewpoint. In addition, it provides useful input to the hydrogeological modelling programme.

Summary

Pore water that resides in the pore space between minerals and along grain boundaries in crystalline rocks of low permeability cannot be sampled by conventional groundwater sampling techniques and therefore has to be characterised by applying indirect methods based on drillcore material. Accessible, interconnected pore water has been successfully extracted by laboratory out-diffusion methods using some 25 drillcore samples from borehole KLX17A with 20 of them being collected along a continuous profile from a water-conducting deformation zone into the intact bedrock matrix. During the Holocene various major periods with different groundwater chemistry (e.g. Glacial, Littorina Sea, Baltic Sea) characterised the fracture waters in the Laxemar subarea to varying depths and extent. This investigation aimed to characterise pore waters along the borehole and also the interaction between stagnant pore water and circulating fracture groundwater. These data can be used to try and resolve the palaeohydrochemical records archived in the pore water.

This report meets the requirements of the SKB internal control document, activity plan “AP PS 400-06-066” (for the ^{36}Cl data “AP PS 400-07-047”) in following the sampling strategy and methodology to extract and analyse the pore water (Table 1-1), and to tabulate the raw analytical data. Interpretation of the data constitutes the next phase of the project.

Included as Appendix A to this report are groundwaters sampled from the water-conducting deformation zone which marked the starting point of the sampled pore water profile. This was carried out as a complement to the pore water studies, but unfortunately was unsuccessful in producing representative groundwater samples. Included as Appendix B are ^{36}Cl age data from selected groundwater types that characterise the Laxemar and Simpevarp subareas within the Oskarshamn site investigation area. The results suggest that groundwaters up to a minimum age of 1.5 Ma may be present in the investigated areas (Appendix B) and this information will be used to support the site description model both hydrochemically and from a palaeohydrogeochemical viewpoint. In addition, it will provide useful input to the hydrogeological modelling programme. In common with the pore water studies, interpretation of the data does not form part of this report and will be presented elsewhere.

Sammanfattning

Porvattnet som återfinns i bergmatrixen påverkar kontinuerligt bergsprickornas cirkulerande grundvatten (vilket i sig avgränsar de lågpermeabla bergspartierna). Omfattningen av porvattnets påverkansgrad beror på de hydrauliska egenskaperna i bergets matrix, på de grundvattenförande sprickorna, på den kemiska gradienten mellan por- och grundvatten, och på hur länge grundvatten har cirkulerat i sprickorna. Porvattenundersökningar i KLX17A, i delområde Laxemar, har som en del av Platsundersökningarna i Oskarshamns hydrogeokemiska programdel utförts för att karaktärisera det porvatten som finns i borrhålet som provtagits och för att förstå samspelet mellan stagnant porvatten och det cirkulerande grundvattnet i sprickorna. Denna undersökning har fokuserats till ett område i borrhålet och där har en provtagningsserie tagits ut från den hydrauliskt aktiva deformationszonen i berget och in i omgivande bergsmatrix.

Porvatten i porutrymmen mellan mineral Korn och kornens bindningar i kristallina bergarter med låg permeabilitet kan inte provtas med för grundvattenprovtagning vanliga metoder utan indirekta metoder baserade på material från borrhålskärnor måste tillämpas. Genom en extraktionsmetodik, så kallad "out-diffusion method" drivs porvattnet ut genom diffusion och detta har analyserats. För denna undersökning har cirka 25 kärnborrhålsprover från KLX17A använts där 20 av dem har tagits i en kontinuerlig serie från en vattenbärande deformationszon i borrhålet och in i den omgivande bergsmatrixen. Under Holocen har flera långa perioder med varierande grundvattensammansättningar (t.ex. Baltiska issjön, Littorinahavet och Östersjön) haft sin påverkan på grundvattnet på olika djup och utsträckning i bergsprickorna i delområde Laxemar. Denna undersökning har syftat till att karaktärisera porvattnet i borrhålet (KLX17A) men även till att se hur det stagnanta porvattnet påverkat grundvattnet i deformationszonen. Dessa grundvattendata kan användas för att försöka förstå de paleohydrokemiska "avtryck" som finns i porvattnet. Denna rapport avhandlar provtagningsstrategi och -metodik för att få ut och analysera porvatten samt redovisar all rådata i tabellform. Tolkning av data ingår inte i denna rapport.

Denna rapport avhandlar endast det som efterfrågas i SKB:s interna kontrolldokument "AP PS 400-06-066" (samt för ^{36}Cl -data "AP PS 400-07-047" (Tabell 1-1), dvs. provtagningsstrategi och metodik för att få ut och analysera porvatten samt redovisa analysresultaten. Utvärdering av analysresultaten ingår inte i denna undersökning.

I Appendix A redovisas resultat från provtagning av grundvatten i den vattenförande deformationszon, som markerar startpunkten för den provtagna porvattenprofilen. Detta utfördes som ett komplement till porvattenstudierna. Emellertid misslyckades försöken att producera representativa grundvattenprover i zonen. Appendix B omfattar ^{36}Cl -data från några utvalda grundvattentyper vilka karaktäriserar delområdena Laxemar och Simpevarp i Oskarshamns platsundersökningsområde. Resultaten antyder att grundvatten upp till minst 1.5 Ma ålder kanske finns i det undersökta området (Appendix B). Denna information kommer att användas för att stödja den platsbeskrivande modellen både från hydrokemisk- och paleohydrogeokemisk synvinkel. Resultaten kommer även att ge användbar information till det hydrogeologiska modellprogrammet. Dessa resultat, precis som med porvattenresultaten, är inte utvärderade då detta inte ingår i denna undersökning.

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1 Introduction

This document reports performance and results of the activity *characterisation of pore water* in drillcore samples within the site investigation programme at Oskarshamn. The drillcore samples were selected during drilling of the telescopic borehole KLX17A; see SKB internal control document, activity plan “AP PS 400-06-066” (Table 1-1).

Crystalline rocks are characterised in general by two hydraulic regimes. The first regime includes the water-conducting zones related to regional or local fracture networks. The second regime includes the bedrock mass of low permeability between the water-conducting zones. Depending on the residence time of fracture groundwater in the water-conducting zones, interaction with water present in the pore space of the low permeable bedrock might become significant. In addition, since repository construction will be restricted largely to bedrock of low permeability, this pore water over time will interact with the repository barrier materials (e.g. bentonite; canister) potentially leading to a deterioration in their physical properties. For safety assessment considerations it is therefore important to know the composition of such pore water and its evolution over recent geological time, certainly during the last thousands to hundreds of thousands of years in accordance with the expected lifespan of a repository. Pore water compositions can be assessed by combining the information gained from pore water profiles within bedrock of low permeability and the chemical and isotopic data of formation groundwaters circulating in the adjacent fracture zones.

Pore water that resides in the interconnected pore space between minerals and along grain boundaries in crystalline rocks of low permeability cannot be sampled by conventional groundwater sampling techniques and therefore has to be characterised by applying indirect methods based on drillcore material. Within the SKB hydrochemical site investigation programme such techniques have been continuously developed and successfully applied to several boreholes at Oskarshamn in the Laxemar subarea /Waber and Smellie, 2006abc/ and Forsmark /Waber and Smellie, 2005, 2008/ to trace the pore water chemistry in low permeable bedrock to depths of around 1,000 metres.

The pore water investigations in borehole KLX17A (Figure 1-1 (map)) aimed to characterise pore waters along the borehole and also the interaction between stagnant pore water and circulating fracture groundwater obtained from a continuously sampled profile from a hydraulically active deformation zone at 99,00–114,00 m depth into the surrounding intact rock matrix (Figure 1-1 (map) and Appendix A). Based on the knowledge obtained from studies performed on boreholes KLX03 and KLX08, detailed mineralogical and fluid inclusion studies otherwise necessary for pore water characterisation, have not been carried out for borehole KLX17A. This report describes the sampling strategy and laboratory methodology employed and tabulates the raw analytical data presented in Chapter 3.

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

Activity plan	Number	Version
Pore space groundwaters in low permeable crystalline rock in KLX17A and KLX13A	AP PS 400-06-066	1.0
Extra analysis of ³⁶ Cl in groundwaters from core drilled and percussion drilled boreholes and Baltic Sea water.	AP PS 400-07-047	1.0

Appended to this report, and of importance when interpreting the palaeohydrogeological significance of the pore waters to the subareas within the Oskarshamn site investigation area, are ^{36}Cl data which help to constrain the age relationships of the fracture groundwaters which are interacting with the pore waters (Figure 1-1 (map) and Appendix B). No samples from borehole KLX17A were included in this study.

This document reports the data/results of pore space groundwaters in KLX17A, which is one of the activities performed within the site investigation at Oskarshamn. The work was carried out in accordance with SKB internal control document, activity plan "AP PS 400-06-066" (Table 1-1).

In Table 1-1 the controlling documents for performing this activity are listed. Both activity plan and method descriptions refer to SKB's internal controlling documents.

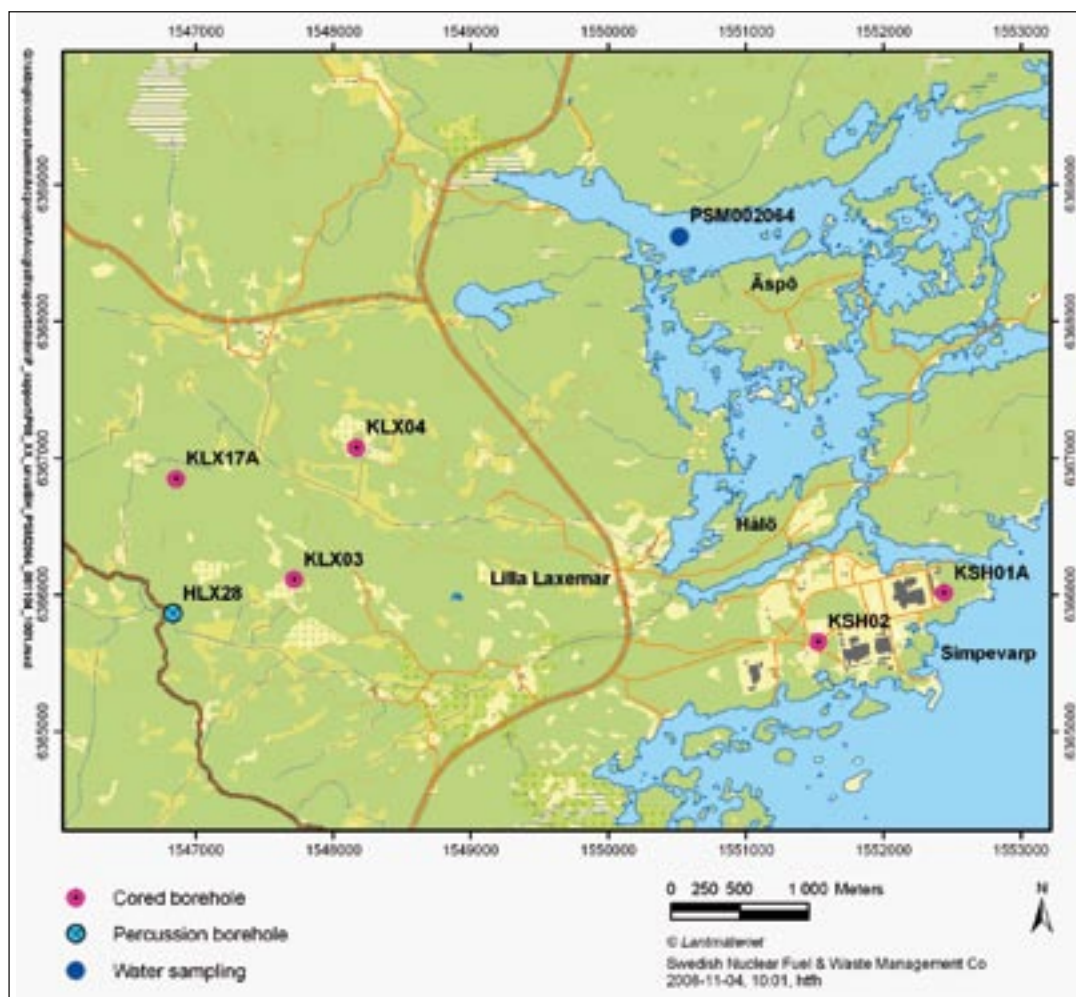


Figure 1-1. Oskarshamn site investigation area showing the location of borehole KLX17A.

2 Materials and methods

From borehole KLX17A drillcore sections of about 30–50 cm in length were sampled between September 16th and October 19th 2006 for pore water characterisation. Category 1 samples were taken at about 100 m intervals along the length of the borehole, and Category 2 samples were continuously sampled perpendicularly from a water-conducting fracture zone into the rock matrix. Sampling commenced when the water-conducting deformation zone EW900 was intercepted at approximately 112 m borehole length during drilling. From this point continuous sampling of 25 samples (Category 2) into the intact rock matrix for a length of 22 m was carried out (i.e. the fracture profile), followed by 5 samples (Category 1) taken at regular depth intervals of about 100 m down to the bottom of the borehole at around 636 m (for sampling details see SKB internal control document, activity plan “AP PS 400-06-066” (Table 1-1) and Figure 2-1 and Table 2-1 below).

From the 22 m long fracture profile the protocol required: 1) complete sampling of the first 5 m of drillcore adjacent to the deformation zone, 2) sampling at small intervals in the following 5 metres, and 3) sampling at increased intervals of a few metres for the final 10 metres. For the 5 deep-seated sections along the borehole, the protocol required the Category 1 samples to be taken from homogeneous, non-fractured bedrock volumes at least 5 metres away from any water-conducting fractures or fracture zones.

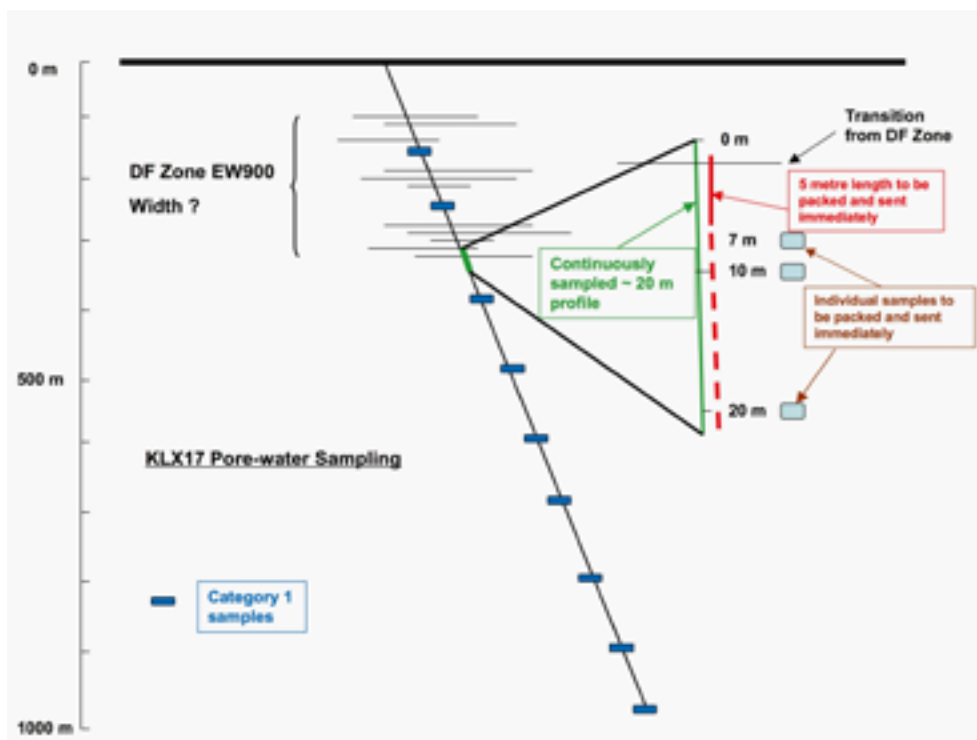


Figure 2-1. Borehole KLX17A: Schematic illustration of the sections planned for pore water sampling along a profile from the deformation zone into the intact rock matrix (fracture profile; Category 2 samples). Category 1 samples were collected at approximately 100 m intervals down to the bottom of the borehole.

An important requirement for pore water characterisation using rock samples is the preservation of the *in-situ* water-saturated state of the rock material immediately following drilling and sampling and during transportation from the site to the laboratory. This precaution is of utmost importance to derive the *in-situ* porosity value for the rock sample not altered by any perturbing effect such as stress release etc /for details see Waber and Smellie, 2008/. Furthermore, it is important to inhibit possible water-rock interactions induced by exposure of the rock sample to air (e.g. oxidation). To minimise these potential perturbing effects the samples were immediately wiped clean with a damp towel following drilling and selection, wrapped in a heavy-duty PVC bag which was repeatedly flushed with nitrogen, evacuated and heat sealed. This procedure was repeated with a second PVC bag and finally sealed in a flushed and evacuated plastic coated Al-foil bag. The samples were then air freighted to the laboratory at the University of Bern, Switzerland, where they were immediately stored at 4°C in a cooling room and prepared for the various measurements and experiments within about 24 hours after arrival.

Once exposed to the air and/or stored over too long a time period, the drillcore samples lose their value for pore-water characterisation. Therefore, all samples received had to be rapidly conditioned so that the different laboratory experimental procedures could be initiated. For the out-diffusion experiments this involved all 25 drillcore samples collected.

Initially, 14 Category 2 samples were selected from the fracture profile for the full analytical programme. In April 2007, it was decided to include the remaining 6 samples from the fracture profile and the 5 Category 1 samples from greater depth for the analyses of $\delta^{18}\text{O}$, $\delta^2\text{H}$ and chloride in pore water. This was based on promising results obtained for the initial 14 samples and the fact that all the deep-seated samples come from large-sized, largely undisturbed blocks of rock matrix based on the BIPS-logging of the borehole /Gustafsson and Gustafsson, 2007/.

2.1 Samples and sample preparation

For legibility reasons the sample labelling adopted in this report is a subsequent numbering of the samples with depth using the borehole name as prefix; similar labelling was used for the laboratory studies. The conversion of this sample description to the SKB sample number and the depth along borehole (borehole length) is given in Table 2-1. The analytical programme performed on the rock samples and experiment solutions is given in Table 2-2.

Drillcore sections sampled close to the deformation zone EW 900 were texturally rather heterogeneous and contained variable amounts of mainly sealed small-sized fractures. In addition, several core sections were broken upon arrival in the laboratory and some Al-bags were slightly inflated (see section 2.4) suggesting that evaporation might have affected the core samples. Because of these inconsistencies, it was necessary to gain some insight into any potential perturbations. This entailed dividing some of the longer sections received into two sub-sections for the out-diffusion experiments in order to obtain some indication of possible perturbations of the samples during storage and transport. These sub-sections were labelled with the sample number followed by an "A" and "B", respectively. In these cases, the rock material used for the isotope diffusive-exchange technique was taken adjacent to sub-sample "B" except for sample KLX17A-3 where this material was taken adjacent to sub-sample "A" (cf. Tables 3-2 and 3-3).

Following arrival at the laboratory the core sections were cut by dry sawing into full-diameter samples of about 12 cm and 19 cm length, respectively, to be used specifically for the out-diffusion experiments. The remaining material from the centre was used for the isotope diffusive-exchange technique and material from the top and bottom of the core section was used for the gravimetric determination of the water content. The wet weight of such material was determined immediately after preparation (within 10 minutes at maximum).

Table 2-1. Borehole KLX17A: List of samples received for pore water studies.

Sample No	SKB Sample No	Sample borehole lengths (m) ¹⁾	Lithology	Alteration / tectonisation	Fissures ²⁾
KLX17A-1	SKB 09748	111.90 – 112.27	Ävrö Granite	high	1 o, 1 c
KLX17A-2	SKB 09749	112.27 – 112.67	Ävrö Granite	high	1 o, 3 c
KLX17A-3	SKB 09750	113.04 – 113.47	Ävrö Granite	high	1 o, 3 c
KLX17A-4	SKB 09751	113.68 – 114.09	Ävrö Granite	moderate	none
KLX17A-5	SKB 09752	114.09 – 114.51	Ävrö Granite	weak	2 c
KLX17A-6	SKB 09753	114.51 – 114.82	Ävrö Granite	weak	none
KLX17A-7	SKB 09754	114.82 – 115.12	Ävrö Granite	weak	1 c
KLX17A-8	SKB 09755	115.12 – 115.61	Ävrö Granite	weak	none
KLX17A-9	SKB 09756	115.63 – 115.98	Ävrö Granite	weak	none
KLX17A-10	SKB 09757	116.04 – 116.29	Ävrö Granite	moderate	1 c
KLX17A-11	SKB 09758	116.29 – 116.64	Ävrö Granite	moderate	2 c
KLX17A-12	SKB 09759	116.64 – 117.04	Ävrö Granite	moderate	2 c
KLX17A-13	SKB 09760	117.04 – 117.31	Ävrö Granite	moderate	2 c
KLX17A-14	SKB 09761	117.45 – 117.95	Ävrö Granite	weak	1 c
KLX17A-15	SKB 09762	117.95 – 118.47	Ävrö Granite	weak	none
KLX17A-16	SKB 09763	118.47 – 118.98	Ävrö Granite	weak	none
KLX17A-17	SKB 09768	120.63 – 121.10	Ävrö Granite	weak	1 c
KLX17A-18	SKB 09775	123.36 – 123.87	Ävrö Granite	weak	none
KLX17A-19	SKB 09790	128.55 – 129.01	Ävrö Granite	weak	none
KLX17A-20	SKB 09802	133.54 – 133.98	Ävrö Granite	weak	none
KLX17A-21	SKB 09803	238.98 – 239.41	Ävrö Granite	weak	none
KLX17A-22	SKB 09804	331.96 – 332.40	Ävrö Granite	weak	1 c
KLX17A-23	SKB 09805	435.49 – 435.94	Ävrö Granite	weak	none
KLX17A-24	SKB 09806	540.15 – 540.61	Ävrö Granite	weak	1 c
KLX17A-25	SKB 09807	635.45 – 635.92	Ävrö Granite	none	none

¹⁾ borehole lengths of drillcore samples received; the average sample length used for the different diffusion experiments might be different (see following tables).

²⁾ aperture of fissures < 1mm; o: open fissure, c: closed fissure.

2.2 Analytical methods

Most of the analytical work of this study has been conducted at the Institute of Geological Sciences, University of Bern, Switzerland. Thus, if not otherwise stated, the analyses have been performed at this institution.

The gravimetric water content, WC_{Grav} , was determined by the gravimetric determination of the water loss by drying sub-samples at 105°C until stable weight conditions (± 0.002 g) were achieved. Such sub-samples included drillcore material specifically designated to water-content measurements, the material used for the isotope diffusive-exchange method, and the large-sized drillcore sections used for the out-diffusion experiments. If the material received allowed it, then the weight of these sub-samples was chosen to be more than about 200 g to minimise possible de-saturation effects and to account for variations in the grain size of the rocks. The mass of the sections used for the out-diffusion experiments ranged between approximately 600 g and 1,100 g and the difference in mass before (i.e. at the time of the sample reception in lab) and after (i.e. after more than 100 days of immersion in the test water) the out-diffusion experiment was less than 0.1 permil for all samples.

Table 2-2. Borehole KLX17A: Experiments and measurements performed on drillcore samples.

Sample	Waterloss porosity	Density	Isotope diffusive exchange	Out-diffusion experiment		
				Chemistry, pH, alkalinity	Sr- and Cl isotopes	Chloride time-series
KLX17-1A	X	X	–	X	P	X
KLX17-1B	X	X	X	X	P	X
KLX17-2A	X	X	–	X	P	X
KLX17-2B	X	X	X	X	P	X
KLX17-3A	X	X	X	X	P	X
KLX17-3B	X	X	–	X	P	X
KLX17-4	X	X	X	X	P	X
KLX17-5A	X	X	–	X	P	X
KLX17-5B	X	X	X	X	P	X
KLX17-6	X	X	X	X	P	X
KLX17-7	X	X	X	X	P	X
KLX17-8A	X	X	–	X	P	X
KLX17-8B	X	X	X	X	P	X
KLX17-9	X	X	X	X	P	X
KLX17-10	X	X	X	X	P	X
KLX17-11	X	X	X	X	P	X
KLX17-12A	X	X	–	X	P	X
KLX17-12B	X	X	X	X	P	X
KLX17-13	X	X	X	X	P	o
KLX17-14A	X	X	–	X	P	o
KLX17-14B	X	X	X	X	P	X
KLX17-15A	X	X	–	X	P	o
KLX17-15B	X	X	X	X	P	o
KLX17-16A	X	X	–	X	P	o
KLX17-16B	X	X	X	X	P	X
KLX17-17	X	X	X	X	P	X
KLX17-18	X	X	X	X	P	–
KLX17-19	X	X	X	X	P	X
KLX17-20	X	X	X	X	P	X
KLX17-21	X	X	X	X	P	X
KLX17-22	X	X	X	X	P	X
KLX17-23	X	X	X	X	P	X
KLX17-24	X	X	X	X	P	X
KLX17-25	X	X	X	X	P	X

X = experiment performed, analyses available.

P = experiment performed, final sample selection and analytical data pending.

o = experiment performed, analyses not performed based on final sample selection.

– = experiment not performed.

NOTE: See section 2.1 for explanation to sample types 'A' and 'B'.

A measure for the bulk wet density of the rocks investigated was obtained from the volume and saturated mass of the core samples used for out-diffusion experiments. The volume was calculated from measurements of height and diameter of the core samples using a vernier calliper with an error of ± 0.01 mm. Variations in the core diameter over the lengths of the samples was found to be less than 0.05 mm for most samples and a constant diameter was used in the calculation of the volume. For the so-derived wet bulk density this results in an error of less than 3%.

The water-loss porosity, WL-P, of the samples was calculated from the average of the different water loss measurements and the volumetrically determined bulk wet density. The stable water isotope composition of the pore water was determined by the isotope diffusive-exchange method adapted to crystalline rocks /for details see Waber and Smellie, 2006b, and Waber and Smellie, 2008/. In this method the isotope exchange occurs through the gaseous phase without any direct contact between the rock sample and the test water. Rock pieces of about 1 cm in diameter from the centre of the core and a small petri dish filled with a test water of known mass isotopic composition are stored together in a vapour-tight glass container. Equilibrium in the three reservoir system, i.e. rock sample, test water and the air inside the container as a diaphragm, is achieved in about 20 to 30 days at room temperature depending on the size and water content of the rock pieces. For each sample two experiments have to be conducted in order to yield the four mass balance equations required to solve the three unknowns, i.e. the $\delta^{18}\text{O}$ and $\delta^2\text{H}$ of the pore water, and the water content of the rock sample. After complete equilibration the test water was removed and analysed by ion-ratio mass spectrometry.

The isotope diffusive-exchange method /Rogge, 1997/ was originally designed for rocks with water contents in the order of several percent. To account for the much lower water content in the crystalline rocks represented by borehole KLX17A, the method was modified in that an artificial test water was used, which is strongly enriched in ^2H and depleted in ^{18}O ($\delta^{18}\text{O} = -109.84\text{‰}$ and $\delta^2\text{H} = +425.5\text{‰}$ V-SMOW). Further, Gaussian error calculations reveal that the accuracy of the experiment depends to a large degree on the ratio of pore water in the rock to test water in the petri dish. In order to reduce the overall error, smaller volumes of test water and larger masses of rock were used for the samples from KLX17A compared to previous experiments conducted on samples from boreholes KLX03 and KLX08 /cf. Waber and Smellie, 2006a and 2006c/.

The isotopic compositions of oxygen and hydrogen in the test solutions were determined by conventional ion-ratio mass spectrometry at Hydroisotop GmbH, Germany. The results are reported relative to the V-SMOW standard with a precision of $\pm 0.15\text{‰}$ for $\delta^{18}\text{O}$ and $\pm 1.5\text{‰}$ for $\delta^2\text{H}$.

If successful, the isotope diffusive-exchange method delivers the stable isotope composition of pore water and the mass of pore water present in the connected pore space of the rock sample. The error of the results was computed for each sample using Gauss' law of error propagation.

Out-diffusion experiments were performed on complete core samples of about 120–190 mm in length by immersion in deionised test water (Figure 2-2). To accelerate the out-diffusion, the vapour-tight PVC containers were placed into a water bath with a constant temperature of 45°C. The weight of the core sample, the experiment container, and the artificial test water used, was measured before and after the experiment to ensure that no loss of test water has occurred during the entire experiment. In addition, weighing of the core before and after the experiment gives valuable information about the saturation state of the core at the beginning of the experiment.

At specific time intervals, initially after a few days and later after a few weeks, 0.5 mL of solution was sampled for the determination of the chloride concentration as a function of time. The small samples were analysed on a Metrohm 861 Compact ion-chromatograph equipped with a CO_2 -Suppressor. The analytical error of these determinations is $\pm 5\%$ based on multiple measurements of the standard solutions.

After steady state with respect to chloride was achieved, i.e. indicated by its levelling out and stabilisation, the core was removed from the container and the solution was immediately analysed for pH and alkalinity (by titration). The remaining solution was split into different aliquots for chemical and isotopic analyses. Major cations and anions were analysed by a conventional Metrohm 861 Compact ion-chromatograph with a relative error of $\pm 5\%$. A blank experiment was also performed in order to evaluate possible contamination by the container and other material used in the experiments.

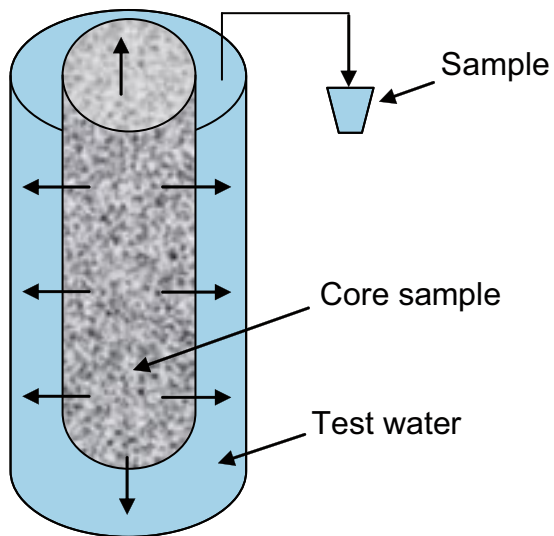


Figure 2-2. Borehole KLX17A: Schematic picture of out-diffusion experiments performed.

2.3 Data handling

All data from this activity are stored in SKB's database Sicada, where they are traceable by the activity plan number "AP PS 400-06-066" (SKB internal control document, Table 1-1).

2.4 Nonconformities

The activity has been performed according to the SKB internal control document, activity plan "AP PS 400-06-066" (Table 1-1). Non-conformities include inadequate packing and/or damage of the sample bags during transport of some samples which led to inflated Al-bags upon arrival of the samples to the laboratory (samples KLX17A-1, -2, -6, -7, -9, -10, -11, -13, -14, -18). A few of these samples obviously suffered evaporation and were excluded from an extended analytical programme. Other samples might have been broken during transport, but had still intact Al-bags (samples KLX17A-3, -4, -16).

3 Results

3.1 Tabulation of analytical data

Table 3-1. Borehole KLX17A: Average values of the gravimetric water content by drying at 105°C (WC_{Grav}), the bulk density, and the water-loss porosity of all investigated drillcore samples.

Laboratory sample No	Lithology	Number of samples	Bulk density wet ¹⁾ (g/cm ³)	WC_{Grav} average (wt.%)	WC_{Grav} 1 σ (wt.%)	WL-P average (Vol.%)	WL-P 1 σ (Vol.%)
KLX17A-1	Ävrö granite	5	2.71	0.575	0.068	1.55	0.18
KLX17A-2	Ävrö granite	5	2.68	0.581	0.090	1.55	0.24
KLX17A-3	Ävrö granite	5	2.66	0.820	0.165	2.15	1.35
KLX17A-4	Ävrö granite	6	2.70	0.625	0.306	1.19	1.08
KLX17A-5	Ävrö granite	5	2.71	0.385	0.191	1.04	0.51
KLX17A-6	Ävrö granite	4	2.86	0.353	0.104	1.00	0.29
KLX17A-7	Ävrö granite	4	2.73	0.300	0.094	0.82	0.26
KLX17A-8	Ävrö granite	6	2.73	0.301	0.067	0.61	0.41
KLX17A-9	Ävrö granite	3	2.73	0.250	0.049	0.68	0.13
KLX17A-10	Ävrö granite	6	2.71	0.308	0.064	0.83	0.17
KLX17A-11	Ävrö granite	5	2.73	0.355	0.098	0.97	0.26
KLX17A-12	Ävrö granite	5	2.72	0.349	0.067	0.95	0.18
KLX17A-13	Ävrö granite	3	2.76	0.321	0.022	0.88	0.06
KLX17A-14	Ävrö granite	5	2.74	0.303	0.036	0.83	0.09
KLX17A-15	Ävrö granite	5	2.72	0.268	0.030	0.73	0.08
KLX17A-16	Ävrö granite	6	2.73	0.246	0.024	0.67	0.07
KLX17A-17	Ävrö granite	5	2.73	0.232	0.045	0.63	0.12
KLX17A-18	Ävrö granite	5	2.85	0.219	0.029	0.62	0.08
KLX17A-19	Ävrö granite	4	2.74	0.254	0.020	0.69	0.05
KLX17A-20	Ävrö granite	5	3.04	0.102	0.013	0.25	0.13
KLX17A-21	Ävrö granite	4	2.74	0.249	0.006	0.68	0.02
KLX17A-22	Ävrö granite	4	2.76	0.239	0.007	0.66	0.02
KLX17A-23	Ävrö granite	4	2.68	0.167	0.008	0.45	0.02
KLX17A-24	Ävrö granite	5	2.70	0.148	0.005	0.40	0.01
KLX17A-25	Ävrö granite	5	2.68	0.140	0.005	0.37	0.01

¹⁾ determined from mass and volume of saturated drillcore samples as received and used for out-diffusion experiment.

Table 3-2. Borehole KLX17A: Gravimetric water content by drying at 105°C (WC_{Grav}), bulk density, and water-loss porosity (WL-P) of drillcore samples used for out-diffusion experiments.

Laboratory sample No	Lithology	Mass drillcore (g)	Bulk density wet ¹⁾ (g/cm ³)	WC _{Grav} average (wt.%)	Error (wt.%)	WL-P average (Vol.%)	Error (Vol.%)
KLX17A-1A	Ävrö granite	630.650	2.71	0.644	0.064	1.74	0.17
KLX17A-1B	Ävrö granite	602.322	2.71	0.609	0.061	1.64	0.16
KLX17A-2A	Ävrö granite	593.100	2.69	0.675	0.068	1.81	0.18
KLX17A-2B	Ävrö granite	564.684	2.68	0.507	0.051	1.36	0.14
KLX17A-3A	Ävrö granite	618.920	2.70	0.522	0.052	1.40	0.14
KLX17A-3B	Ävrö granite	585.795	2.62	1.725	0.173	4.47	0.45
KLX17A-4	Ävrö granite	999.100	2.70	0.637	0.064	1.71	0.17
KLX17A-5A	Ävrö granite	618.520	2.71	0.520	0.052	1.40	0.14
KLX17A-5B	Ävrö granite	632.063	2.71	0.269	0.027	0.73	0.07
KLX17A-6	Ävrö granite	631.300	2.86	0.369	0.037	1.05	0.11
KLX17A-7	Ävrö granite	617.583	2.73	0.295	0.030	0.81	0.08
KLX17A-8A	Ävrö granite	630.555	2.73	0.268	0.027	0.73	0.07
KLX17A-8B	Ävrö granite	630.110	2.73	0.295	0.030	0.81	0.08
KLX17A-9	Ävrö granite	631.526	2.73	0.297	0.030	0.81	0.08
KLX17A-10	Ävrö granite	584.832	2.71	0.410	0.041	1.11	0.11
KLX17A-11	Ävrö granite	645.167	2.73	0.256	0.026	0.70	0.07
KLX17A-12A	Ävrö granite	622.750	2.70	0.370	0.037	1.00	0.10
KLX17A-12B	Ävrö granite	624.615	2.73	0.303	0.030	0.83	0.08
KLX17A-13	Ävrö granite	632.414	2.76	0.313	0.031	0.86	0.09
KLX17A-14A	Ävrö granite	635.941	2.73	0.364	0.036	0.99	0.10
KLX17A-14B	Ävrö granite	623.175	2.76	0.292	0.029	0.80	0.08
KLX17A-15A	Ävrö granite	643.280	2.74	0.279	0.028	0.76	0.08
KLX17A-15B	Ävrö granite	1,001.724	2.71	0.274	0.027	0.74	0.07
KLX17A-16A	Ävrö granite	636.419	2.72	0.265	0.027	0.72	0.07
KLX17A-16B	Ävrö granite	632.105	2.74	0.250	0.025	0.69	0.07
KLX17A-17	Ävrö granite	1,008.440	2.73	0.249	0.025	0.68	0.07
KLX17A-18	Ävrö granite	1,036.583	2.85	0.242	0.024	0.69	0.07
KLX17A-19	Ävrö granite	1,012.750	2.74	0.248	0.025	0.68	0.07
KLX17A-20	Ävrö granite	1,110.530	3.04	0.097	0.010	0.26	0.03
KLX17A-21	Ävrö granite	1,016.900	2.74	0.254	0.025	0.69	0.07
KLX17A-22	Ävrö granite	1,038.180	2.76	0.231	0.023	0.64	0.06
KLX17A-23	Ävrö granite	1,015.649	2.68	0.171	0.017	0.46	0.05
KLX17A-24	Ävrö granite	1,007.412	2.70	0.146	0.015	0.39	0.04
KLX17A-25	Ävrö granite	998.973	2.68	0.140	0.014	0.38	0.04

¹⁾ determined from mass and volume of saturated drillcore sample as received and used for out-diffusion experiment.

Table 3-3. Borehole KLX17A: Water content derived by the isotope diffusive exchange method.

Laboratory sample No	Borehole length (m)	Lithology	WC _{IsoExch} ¹⁾ (wt.%)	Error WC _{IsoExch} ^{1) 2)} (wt.%)
KLX17A-1A	111.98	Ävrö granite	–	–
KLX17A-1B	112.19	Ävrö granite	0.485	0.008
KLX17A-2A	112.35	Ävrö granite	–	–
KLX17A-2B	112.60	Ävrö granite	0.612	0.007
KLX17A-3A	113.12	Ävrö granite	0.508	0.007
KLX17A-3B	113.39	Ävrö granite	–	–
KLX17A-4	113.79	Ävrö granite	0.447	0.006
KLX17A-5A	114.17	Ävrö granite	–	–
KLX17A-5B	114.43	Ävrö granite	0.210	0.005
KLX17A-6	114.59	Ävrö granite	0.537	0.007
KLX17A-7	114.90	Ävrö granite	0.243	0.007
KLX17A-8A	115.20	Ävrö granite	–	–
KLX17A-8B	115.53	Ävrö granite	0.401	0.005
KLX17A-9	115.71	Ävrö granite	0.218	0.005
KLX17A-10	116.12	Ävrö granite	0.242	0.005
KLX17A-11	116.37	Ävrö granite	0.349	0.006
KLX17A-12A	116.72	Ävrö granite	–	–
KLX17A-12B	116.96	Ävrö granite	0.307	0.005
KLX17A-13	117.12	Ävrö granite	exp. failed	exp. failed
KLX17A-14A	117.53	Ävrö granite	–	–
KLX17A-14B	117.87	Ävrö granite	0.289	0.005
KLX17A-15A	118.03	Ävrö granite	–	–
KLX17A-15B	118.36	Ävrö granite	0.258	0.005
KLX17A-16A	118.55	Ävrö granite	–	–
KLX17A-16B	118.90	Ävrö granite	0.250	0.005
KLX17A-17	120.74	Ävrö granite	0.193	0.004
KLX17A-18	123.47	Ävrö granite	exp. failed	exp. failed
KLX17A-19	128.66	Ävrö granite	0.240	0.004
KLX17A-20	133.65	Ävrö granite	0.107	0.003
KLX17A-21	239.09	Ävrö granite	0.229	0.004
KLX17A-22	332.07	Ävrö granite	0.254	0.004
KLX17A-23	435.61	Ävrö granite	exp. failed	exp. failed
KLX17A-24	540.26	Ävrö granite	0.159	0.004
KLX17A-25	635.56	Ävrö granite	0.222	0.020

¹⁾ = experiment not performed; exp. failed = experiment failed due to de-saturated sample (cf. section 2.4) and/or leakage of experiment container (sample KLX17A-23).

²⁾ error calculated with Gauss' law of error propagation.

Table 3-4:1(5). Borehole KLX17A: Chemical composition of solutions from out-diffusion experiments at steady state conditions.

Out-Diffusion Experiment Solution	Units	KLX17A-1A	KLX17A-1B	KLX17A-2A	KLX17A-2B	KLX17A-3A	KLX17A-3B	KLX17A-4	KLX17A-5A
Sample description									
Borehole Length	m	111.98	112.19	112.35	112.60	113.12	113.39	113.79	114.17
Rock Type		Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite
Water-Rock Ratio	mass	0.129	0.132	0.143	0.155	0.129	0.148	0.120	0.128
Experiment Temperature	°C	45	45	45	45	45	45	45	45
Experiment Time	days	106	106	106	106	106	106	106	106
Misc. Properties									
Chemical Type		<u>Na-Ca-HCO₃</u>	<u>Na-Ca-HCO₃</u>	<u>Na-Ca-HCO₃</u>	<u>Na-Ca-HCO₃</u>	<u>Na-Ca-HCO₃</u>	<u>Na-Ca-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>
pH	-log(H ⁺)	7.39	7.4	7.42	7.34	7.34	7.29	7.4	7.34
Sample Temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na ⁺)	mg/L	82.1	85.6	87.8	68.7	91.4	96.8	129.0	123.6
Potassium (K ⁺)	mg/L	3.9	3.2	3.3	3.6	4.8	3.8	4.5	4.3
Magnesium (Mg ⁺²)	mg/L	4.1	4.6	3.3	4.0	3.6	3.8	2.0	1.5
Calcium (Ca ⁺²)	mg/L	31.6	33.4	25.1	34.5	31.0	27.1	22.1	13.9
Strontium (Sr ⁺²)	mg/L	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0
Anions									
Fluoride (F ⁻)	mg/L	2.1	3.5	4.3	3.8	2.9	2.8	5.1	6.1
Chloride (Cl ⁻)	mg/L	4.4	4.2	3.2	3.2	3.9	6.9	4.0	3.6
Bromide (Br ⁻)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Sulphate (SO ₄ ⁻²)	mg/L	16.7	5.4	3.4	3.1	3.7	9.6	8.2	15.4
Nitrate (NO ₃ ⁻)	mg/L	< 0.5	< 0.5	< 0.5	1.4	< 0.5	0.7	< 0.5	< 0.5
Total Alkalinity as HCO ₃ ⁻	mg/L	267.9	277.6	270.9	245.9	286.8	297.8	332.5	294.7
Oxalate (C ₂ O ₄ ⁻²)	mg/L	10	10	5	5	10	5	15	10
Neutral species									
Silica (Si)	mg/L	11.0	10.2	7.9	9.2	9.5	4.7	9.4	9.4
Calc. Parameters									
Total dissolved solids	mg/L	434	438	414	382	448	459	532	483
Charge Balance	%	3.56%	5.93%	4.41%	6.28%	6.00%	3.66%	4.84%	4.10%

Table 3-4:2(5).

Out-Diffusion Experiment Solution	Units	KLX17A-5B	KLX17A-6	KLX17A-7	KLX17A-8A	KLX17A-8B	KLX17A-9	KLX17A-10	KLX17A-11
Sample description									
Borehole Length	m	114.43	114.59	114.90	115.20	115.53	115.71	116.12	116.37
Rock Type		Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite
Water-Rock Ratio	mass	0.121	0.140	0.170	0.168	0.128	0.163	0.143	0.138
Experiment Temperature	°C	45	45	45	45	45	45	45	45
Experiment Time	days	106	106	106	106	106	106	106	106
Misc. Properties									
Chemical Type		<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>
pH	-log(H ⁺)	7.51	7.57	7.49	7.48	7.35	7.55	7.49	7.52
Sample Temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na ⁺)	mg/L	118.5	129.3	93.0	89.1	123.0	82.8	187.0	87.9
Potassium (K ⁺)	mg/L	4.6	3.4	4.1	4.3	5.3	3.5	3.2	3.9
Magnesium (Mg ⁺²)	mg/L	1.2	0.8	0.6	<0.5	1.0	0.8	0.8	0.8
Calcium (Ca ⁺²)	mg/L	17.3	13.2	17.4	15.0	21.6	13.2	13.3	20.1
Strontium (Sr ⁺²)	mg/L	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0
Anions									
Fluoride (F ⁻)	mg/L	5.2	5.6	4.7	5.0	4.7	5.2	6.8	4.4
Chloride (Cl ⁻)	mg/L	3.3	3.8	2.9	3.7	6.0	4.0	3.9	3.6
Bromide (Br ⁻)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Sulphate (SO ₄ ⁻²)	mg/L	17.9	7.2	8.1	11.4	8.3	5.3	6.9	5.3
Nitrate (NO ₃ ⁻)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	1.2
Total Alkalinity as HCO ₃ ⁻	mg/L	291.1	317.9	250.8	227.6	305.7	207.5	427.1	245.9
Oxalate (C ₂ O ₄ ⁻²)	mg/L	10	5	5	5	20	10	20	2
Neutral species									
Silica (Si)	mg/L	11.3	9.3	9.5	9.9	10.7	9.4	10.3	8.6
Calc. Parameters									
Total dissolved solids	mg/L	481	496	396	372	507	342	680	383
Charge Balance	%	4.09%	4.52%	3.54%	3.28%	4.66%	3.31%	5.13%	4.78%

Table 3-4:3(5).

Out-Diffusion Experiment Solution	Units	KLX17A-12A	KLX17A-12B	KLX17A-13	KLX17A-14A	KLX17A-14B	KLX17A-15A	KLX17A-15B	KLX17A-16A
Sample description									
Borehole Length	m	116.72	116.96	117.12	117.53	117.87	118.03	118.36	118.55
Rock Type		Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite
Water-Rock Ratio	mass	0.137	0.131	0.162	0.173	0.127	0.123	0.114	0.160
Experiment Temperature	°C	45	45	45	45	45	45	45	45
Experiment Time	days	106	106	106	106	106	106	106	106
Misc. properties									
Chemical Type		<u>Na- HCO₃</u>	<u>Na- HCO₃</u>	<u>Na- HCO₃</u>	<u>Na-(Ca)- HCO₃</u>	<u>Na-(Ca)- HCO₃</u>	<u>Na-(Ca)- HCO₃</u>	<u>Na-(Ca)- HCO₃</u>	<u>Na-Ca- HCO₃</u>
pH	-log(H ⁺)	7.42	7.35	7.14	7.55	7.59	7.49	7.39	7.43
Sample Temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na ⁺)	mg/L	129.5	140.8	96.4	109.3	128.0	120.7	116.6	108.1
Potassium (K ⁺)	mg/L	4.5	4.4	2.5	3.6	4.0	5.6	6.1	5.3
Magnesium (Mg ⁺²)	mg/L	0.6	0.9	0.0	0.8	0.6	1.4	1.4	1.0
Calcium (Ca ⁺²)	mg/L	10.3	12.5	5.0	15.3	14.5	23.5	23.3	26.8
Strontium (Sr ⁺²)	mg/L	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0	< 1.0
Anions									
Fluoride (F ⁻)	mg/L	7.9	7.1	8.8	6.2	5.9	4.7	4.1	3.9
Chloride (Cl ⁻)	mg/L	3.9	4.6	3.1	3.8	5.4	6.0	7.7	5.2
Bromide (Br ⁻)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Sulphate (SO ₄ ⁻²)	mg/L	8.0	19.4	15.0	10.1	11.0	17.3	13.4	14.3
Nitrate (NO ₃ ⁻)	mg/L	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
Total Alkalinity as HCO ₃ ⁻	mg/L	283.7	300.2	191.0	302.0	311.8	283.7	321.6	274.0
Oxalate (C ₂ O ₄ ⁻²)	mg/L	15	20	10	5	5	10	5	10
Neutral species									
Silica (Si)	mg/L	11.3	13.3	11.5	10.1	10.6	11.1	11.7	10.5
Calc. Parameters									
Total dissolved solids	mg/L	475	523	343	467	497	484	511	459
Charge Balance	%	5.24%	4.87%	3.22%	-0.28%	4.22%	8.31%	3.27%	7.58%

Table 3-4:4(5).

Out-Diffusion Experiment Solution	Units	KLX17A-16B	KLX17A-17	KLX17A-18	KLX17A-19	KLX17A-20	KLX17A-21	KLX17A-22	KLX17A-23
Sample description									
Borehole Length	m	118.90	120.74	123.47	128.66	133.65	239.09	332.07	435.61
Rock Type		Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	Ävrö Granite	
Water-Rock Ratio	mass	0.128	0.114	0.115	0.118	0.106	0.101	0.108	0.115
Experiment Temperature	°C	45	45	45	45	45	45	45	45
Experiment Time	days	106	106	106	106	106	106	106	124
Misc. Properties									
Chemical Type		<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>	<u>Na-(Ca)-HCO₃</u>
pH (lab)	-log(H ⁺)	7.49	7.41	7.64	7.5	7.34	7.52	7.29	7.34
Sample Temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na ⁺)	mg/L	104.5	124.2	143.8	129.3	124.1	127.3	120.6	71.2
Potassium (K ⁺)	mg/L	4.4	6.0	5.4	4.6	7.2	3.4	4.1	2.8
Magnesium (Mg ⁺²)	mg/L	1.0	0.9	0.7	0.7	1.9	0.3	0.9	0.3
Calcium (Ca ⁺²)	mg/L	18.2	18.6	14.5	14.9	23.7	9.5	17.2	8.6
Strontium (Sr ⁺²)	mg/L								
Anions									
Fluoride (F ⁻)	mg/L	4.4	4.1	4.4	4.0	0.7	3.7	3.8	6.5
Chloride (Cl ⁻)	mg/L	4.9	6.3	5.5	6.5	2.2	7.9	14.4	10.6
Bromide (Br ⁻)	mg/L								
Sulphate (SO ₄ ⁻²)	mg/L	10.4	10.2	17.0	6.2	36.7	6.9	12.4	15.7
Nitrate (NO ₃ ⁻)	mg/L								4.8
Total Alkalinity as HCO ₃ ⁻	mg/L	276.4	319.7	339.9	326.4	311.8	295.9	274.6	156.2
Oxalate (C ₂ O ₄ ⁻²)	mg/L	5	5	10	5	15	5	15	< 1.0
Neutral species									
Silica (Si)	mg/L	10.2	12.4	9.3	11.3	9.6	9.9	12.1	-
Calc. Parameters									
Total dissolved solids	mg/L	440	508	551	509	533	470	475	272
Charge Balance	%	3.79%	4.74%	4.60%	4.43%	4.53%	5.10%	4.73%	0.19%

Table 3-4:5(5).

Out-Diffusion Experiment Solution	Units	KLX17A-24	KLX17A-25	Blank Solution
Sample description				
Borehole length	m	540.26	635.56	
Rock Type		Ävrö Granite	Ävrö Granite	
Water-Rock Ratio	mass	0.108	0.111	
Experiment Temperature	°C	45	45	45
Experiment Time	days	124	124	106
Misc. Properties				
Chemical Type		Na-Ca- <u>HCO₃</u> -SO ₄ -Cl	Ca-Na- SO ₄ -Cl	
pH (lab)	-log(H ⁺)	7.26	6.88	
Sample Temperature	°C	20	20	20
Cations				
Sodium (Na ⁺)	mg/L	109.5	94.5	0.2
Potassium (K ⁺)	mg/L	8.9	7.4	< 0.1
Magnesium (Mg ⁺²)	mg/L	1.0	1.2	0.3
Calcium (Ca ⁺²)	mg/L	74.7	269.1	0.1
Strontium (Sr ⁺²)	mg/L	< 1.0	< 1.0	
Anions				
Fluoride (F ⁻)	mg/L	3.3	2.6	< 0.1
Chloride (Cl ⁻)	mg/L	91.5	62.2	0.1
Bromide (Br ⁻)	mg/L	1.4	1.0	< 0.1
Sulphate (SO ₄ ⁻²)	mg/L	126.0	639.3	< 0.1
Nitrate (NO ₃ ⁻)	mg/L	< 0.5	0.9	
Total Alkalinity as HCO ₃ ⁻	mg/L	192.2	83.6	< 1.0
Oxalate (C ₂ O ₄ ⁻²)	mg/L	< 1.0	< 1.0	< 1.0
Neutral species				
Silica (Si)	mg/L	–	–	
Calc. Parameters				
Total dissolved solids	mg/L	608	1,161	< 10
Charge Balance	%	1.47%	3.56%	

Table 3-5: Borehole KLX17A: Chloride concentration of pore water calculated from out-diffusion solutions and the water content of the corresponding large-sized drillcore sample.

Laboratory sample No	Borehole length (m)	Comment	Pore water Cl (mg/kg H ₂ O)	Pore water Cl + error ¹⁾ (mg/kg H ₂ O)	Pore water Cl - error ¹⁾ (mg/kg H ₂ O)
KLX17A-1A					
KLX17A-1B	112.09	average A and B	91	10	8
KLX17A-2A	–		–	–	–
KLX17A-2B	112.47	average A and B	81	9	7
KLX17A-3A	113.26	average A and B	70	7	6
KLX17A-3B	–	–	–	–	–
KLX17A-4	113.89	–	77	8	7
KLX17A-5A	–	–	–	–	–
KLX17A-5B	114.3	average A and B	107	12	9
KLX17A-6	114.67	–	143	15	13
KLX17A-7	114.97	–	161	18	14
KLX17A-8A	–	–	–	–	–
KLX17A-8B	115.37	–	253	28	23
KLX17A-9	115.81	–	215	23	19
KLX17A-10	116.17	–	180	20	16
KLX17A-11	116.47	–	188	20	17
KLX17A-12A	–	–	–	–	–
KLX17A-12B	116.84	–	161	17	14
KLX17A-13	117.18	–	151	16	13
KLX17A-14A	–	–	–	–	–
KLX17A-14B	117.7	–	204	22	18
KLX17A-15A	–	–	–	–	–
KLX17A-15B	118.21	–	278	30	25
KLX17A-16A	–	–	–	–	–
KLX17A-16B	118.73	–	275	30	25
KLX17A-17	120.87	–	287	31	25
KLX17A-18	123.62	–	252	27	22
KLX17A-19	128.78	–	310	34	28
KLX17A-20	133.76	–	235	26	21
KLX17A-21	239.2	–	315	34	28
KLX17A-22	332.18	–	680	74	61
KLX17A-23	435.72	–	709	78	64
KLX17A-24	540.38	–	6,823	748	612
KLX17A-25	635.69	–	4,960	544	445

¹⁾ error based on $\pm 10\%$ uncertainty in the water-loss measurement.

Table 3-6. Borehole KLX17A: $\delta^{18}\text{O}$ and $\delta^2\text{H}$ of pore water derived from the isotope diffusive-exchange method.

Laboratory sample No	Average bore-hole length (m)	Pore Water $\delta^{18}\text{O}$ ¹⁾ (‰ V-SMOW)	Error $\delta^{18}\text{O}$ ²⁾ (‰ V-SMOW)	Pore Water $\delta^2\text{H}$ ¹⁾ (‰ V-SMOW)	Error $\delta^2\text{H}$ ²⁾ (‰ V-SMOW)
KLX17A-1A	111.98	–	–	–	–
KLX17A-1B	112.19	–9.49	0.55	–74.3	4.7
KLX17A-2A	112.35	–	–	–	–
KLX17A-2B	112.60	–10.53	0.38	–79.9	3.3
KLX17A-3A	113.12	–10.46	0.46	–79.6	4.1
KLX17A-3B	113.39	–	–	–	–
KLX17A-4	113.79	–10.10	0.43	–79.1	3.9
KLX17A-5A	114.17	–	–	–	–
KLX17A-5B	114.43	–9.92	1.01	–75.3	8.7
KLX17A-6	114.59	–9.74	0.47	–75.3	3.9
KLX17A-7	114.90	–9.76	1.01	–75.1	9.7
KLX17A-8A	115.20	–	–	–	–
KLX17A-8B	115.53	–9.62	0.85	–76.6	7.1
KLX17A-9	115.71	–9.97	1.04	–80.6	8.9
KLX17A-10	116.12	–10.00	0.91	–82.4	7.6
KLX17A-11	116.37	–10.90	0.65	–83.4	5.4
KLX17A-12A	116.72	–	–	–	–
KLX17A-12B	116.96	–11.38	0.69	–86.8	6.0
KLX17A-13	117.53	exp. failed		exp. failed	
KLX17A-14A	117.87	–	–	–	–
KLX17A-14B	118.03	–11.22	0.67	–74.8	5.6
KLX17A-15A	118.36	–	–	–	–
KLX17A-15B	118.55	–10.64	0.87	–89.0	7.9
KLX17A-16A	118.90	–	–	–	–
KLX17A-16B	120.74	–10.68	0.96	–90.1	7.5
KLX17A-17	123.47	–10.62	0.94	–89.8	8.0
KLX17A-18	128.66	exp. failed		exp. failed	
KLX17A-19	133.65	–7.86	0.85	–82.2	6.6
KLX17A-20	239.09	–7.58	1.80	–84.1	12.7
KLX17A-21	332.07	–10.96	0.80	–96.5	6.7
KLX17A-22	435.61	–12.82	0.72	–97.8	5.9
KLX17A-23	540.26	exp. failed		exp. failed	
KLX17A-24	635.56	–5.07	1.30	–34.5	9.9
KLX17A-25	111.98	–4.79	1.47	–37.6	15.8

¹⁾ – = experiment not performed; exp. failed = experiment failed due to de-saturated sample (cf. section 2.4) and/or leakage of experiment container (sample KLX17A-23).

²⁾ cumulated error calculated with Gauss' law of error propagation; analytical error on the individual determination is $\pm 0.15\text{‰}$ for $\delta^{18}\text{O}$ and $\pm 1.5\text{‰}$ for $\delta^2\text{H}$.

4 Conclusions

This report meets the requirements of the SKB internal control document, activity plan “AP PS 400-06-066” (Table 1-1) in following the sampling strategy and methodology to extract and analyse the pore water, and to tabulate the raw analytical data. Interpretation of the data constitutes the next phase of the project and will be reported elsewhere.

Also appended to this report is the chemistry of the groundwater sampled from the deformation zone which intersects the KLX17A borehole at 99.00–114.00 m borehole length (see Appendix A). Unfortunately, because of the near-surface location and short-circuiting via interconnected fracture networks, the sampling of representative groundwater was unsuccessful (category 5 in quality) and therefore should not be used.

Furthermore, ^{36}Cl age data has been compiled from selected groundwater types that characterise the Laxemar and Simpevarp subareas within the Oskarshamn site investigation area (see Appendix B). The results indicate that groundwaters possibly up to a minimum age of 1.5 Ma may be present and this information will be used to support the site description model both hydrochemically and from a palaeohydrogeochemical viewpoint. In addition, it will provide useful input to the hydrogeological modelling programme. In common with the pore water, interpretation of these data does not form part of this report and will be presented elsewhere.

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The ^{36}Cl analyses were carried out at the Purdue Rare Isotope Measurement Laboratory (PRIME Lab), University of Perdue, USA, under the direction of Professor Marc Caffee.

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Appendix A

Fracture groundwater chemical data (KLX17A: 99.00–114.00 m)

The groundwater chemistry of the sampled deformation zone in KLX17A (borehole section length 99.00–114.00 m) is presented below in Table A-1.

Note: Unfortunately, because of the near-surface location and short-circuiting via interconnected fracture networks, the sampling of representative groundwater was unsuccessful (category 5 in quality) and therefore should not be used.

Table A-1. Borehole KLX17A: Chemistry of groundwater from section 99.00–114.00 m.

Borehole	KLX17A
SKB Sampled No.	15,154
Sampled	2007/10/18
Secup	99.00
Seclow	114.00
Secmid	106.50
Charge Balance (±%)	1.58
Sodium (mg/L)	84.3
Potassium (mg/L)	1.16
Calcium (mg/L)	11.20
Magnesium (mg/L)	22.00
Bicarbonate (mg/L)	243.00
Chloride (mg/L)	6.20
Sulphate (mg/L)	6.42
Sulphate-S (mg/L)	2.37
Bromide (mg/L)	-0.200
Silica (mg/L)	7.98
Lithium (mg/L)	0.008
Strontium (mg/L)	0.179
¹⁸ O (‰ V-SMOW)	-10.70
Deuterium (‰ V-SMOW)	-75.5

³⁶Cl data from groundwaters selected from subareas within the Oskarshamn site investigation area

Some ³⁶Cl data already exist for the Laxemar and Äspö subareas within the Oskarshamn site investigation area /Louvaton et al. 1999/; this has now been supplemented (Table B-1) by selecting additional groundwater samples from the Laxemar-Simpevarp area. Selection was based on specific and reliable groundwater types that describe the Laxemar-Simpevarp area. By dating these groundwaters their residence times can be better constrained.

Table B-1. ³⁶Cl data for selected strategic groundwaters from subareas within the Oskarshamn site investigation area.

Sample	Depth (m)	Cl (mg/L)	at. ³⁶ Cl/at.Cl ± Error	Error (%)	Origin	SKB No.
PSM002064	6.50–7.50	3,500–3,800	$1.7 \cdot 10^{-15} \pm 1.6 \cdot 10^{-15}$	96	Baltic Sea	11515
HLX28	~ 80	< 50	$76 \cdot 10^{-15} \pm 5 \cdot 10^{-15}$	6	Fresh meteoric recharge	10894
KSH01A	238–277	6,500	$26 \cdot 10^{-15} \pm 4 \cdot 10^{-15}$	17	Brackish marine (Littorina)	11494
KLX04	971.21–976.21	8,000	$48 \cdot 10^{-15} \pm 4 \cdot 10^{-15}$	8	Brackish non-marine	7753
KLX03	964–975	10,000	$32 \cdot 10^{-15} \pm 4 \cdot 10^{-15}$	12	Saline	10077
KSH02	955–963	17,000	$39 \cdot 10^{-15} \pm 7 \cdot 10^{-15}$	19	Saline	7114

at. = atomic weight.