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Oskarshamn site investigation

Borehole KLX08 Characterisation of pore water

Part 1: Methodology and analytical data

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August 2006

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the authors and do not necessarily coincide with those of the client.

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Abstract

Drillcore material has been successfully sampled from borehole KLX08 for studies relating to the characterisation of pore water that resides in the connected pore space. The methodology to extract and analyse the pore water is outlined and the raw analytical data are tabulated.

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 extracted successfully by laboratory out-diffusion methods using some 19 drillcore samples from borehole KLX08 as part of the Oskarshamn hydrogeochemical site investigation programme. The objective was to characterise these pore waters chemically and isotopically and relate these data to the present and past groundwater evolution of the site. This report outlines the methodology to extract and analyse the pore water and tabulates the raw analytical data.

Sammanfattning

Porvatten som uppehåller sig i porutrymmen mellan mineral och längs mineralkornsgränser i kristallint berg med låg permeabilitet kan inte provtas med konventionella provtagnings-tekniker för grundvatten och måste därför karakteriseras genom att använda indirekta metoder baserade på borrhärnmaterial. Tillgängligt, sammanbundet porvatten har framgångsrikt extraherats på laboratorium med hjälp av diffusionsmetoder på 19 stycken borrhärnprover från borrhål KLX08 som en del i det hydrogeokemiska platsundersökningsprogrammet i Oskarshamn. Syftet var att karakterisera dessa porvatten kemiskt och isotopiskt och att relatera dessa data till platsens nutida och dåtida grundvattenutveckling. Denna rapport sammanfattar metodiken för att extrahera och analysera porvattnet och tabellerar analysrådatan.

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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 KLX08; see controlling document AP PS 400-05-008.

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 formation 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 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. In the recent past such techniques have been continuously developed and tested /Smellie et al. 2003, Waber and Smellie 2004/ until finally applied to borehole KFM06A at Forsmark /Waber and Smellie 2005/ and to borehole KLX03 in the Laxemar subarea to trace the pore water chemistry in low permeable bedrock to depths of around 1,000 m /Waber and Smellie 2006ab/.

A similar approach has been carried out for borehole KLX08. The methodology employed for pore water extraction and the resulting analytical data are reported in this present report; preliminary interpretation of the data has been reported in /SKB 2006/ and final reporting will be as a P-Report Part 2. Note that it was not necessary to carry out detailed mineralogical and fluid inclusion studies in borehole KLX08, since the main rock types are similar to those already characterised in borehole KLX03. Such data are necessary for pore water characterisation.

2 Materials and methods

From borehole KLX08 25 drillcore sections were sampled between April 8th and June 12th 2005 for pore water characterisation. The sections of about 20–50 cm in length were taken at regular depth intervals of approximately 50 m (for details see AP PS 400-05-008). The sampling procedure required the samples to be taken from homogeneous, non-fractured bedrock volumes at least 5 m away from any water-conducting fractures or fracture zones. To safeguard against the selection of unsuitable samples, which might not be obvious at the time, extra core lengths were taken during drilling when good rock properties were observed.

An important requirement for pore water characterisation using rock samples is the preservation of the fully water-saturated state of the rock material immediately following drilling and sampling and during transportation from the site to the laboratory. This precaution is to inhibit possible water-rock interactions induced by exposure of the rock sample to air. To minimise these potential perturbing effects the samples were immediately wiped clean with a dry towel following drilling and selection, wrapped into 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 repeated and sealed in a plastic coated Al-foil. 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 20 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 19 of the 25 samples received; the 6 samples discarded are listed in Table 2-1. These 6 samples were collected in the hope that they represented a fracture profile, but this was not to be the case and so there was no need to include them in the investigation.

In November 2005 a final decision was made as to which of the 19 samples involved in the on-going out-diffusion experiments were considered most suitable for future interpretation. This selection initially was based on a personal on-site drillcore inspection, use of available drillcore mapping information, BIPS logs and also hydraulic data from downhole differential flow measurements. Guidance of the field personnel was invaluable. Ten samples were selected for the full analytical programme. In February 2006, it was decided to include an additional 9 samples for the analyses of $\delta^{18}\text{O}$, $\delta^2\text{H}$ and Cl in the pore waters. This was based on promising results obtained for the previous initially selected ten samples and the fact that almost all samples came from largely undisturbed zones.

Table 2-1. Borehole KLX08: List of samples discarded from the pore water investigations.

SKB sample number	Sample length	Comment
9703	200.45–200.80	Not representative of a fracture profile
9704	201.21–201.47	Not representative of a fracture profile
9705	201.47–201.76	Not representative of a fracture profile
9706	202.30–202.65	Not representative of a fracture profile
9707	203.07–203.65	Not representative of a fracture profile
9708	203.65–204.00	Not representative of a fracture profile

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 vertical depth along borehole is given in Table 2-2. The analytical programme performed on the rock samples and experiment solutions is given in Table 2-3.

Following arrival at the laboratory the core sections were cut by dry sawing into full-diameter samples of about 19 cm length to be used specifically for the out-diffusion experiments. The remaining material from the top and bottom of the core section was used for the isotope diffusive-exchange method and the determination of the water content. For these methods the outer rim of the core (~ 0.5 cm) was first removed by chisel and hammer to minimise any small-scale sample effects resulting from de-saturation during initial perturbations by drilling activities and subsequent sample preparation. The wet weight of such material was determined immediately after preparation.

Table 2-2. Borehole KLX08: List of samples used for pore-water studies.

Sample no	SKB sample no	Average depth along borehole (m)	Lithology	Alteration/ tectonisation ¹⁾	Fracture intensity (per metre)
KLX08-1	SKB 09700	150.22	Avrö granite	± 1.6 m	8–9
KLX08-2	SKB 09701	199.45	Fine-grained granite	± 1.0 m	7–8
KLX08-3	SKB 09702	200.26	Avrö granite	± 1.5 m	7–8
KLX08-4	SKB 09709	250.19	Avrö granite	± 13 m	4–5
KLX08-5	SKB 09710	302.34	Avrö granite	± 1.2 m	9–10
KLX08-6	SKB 09711	347.10	Avrö granite	± 37 m	2–3
KLX08-7	SKB 09712	395.65	Avrö granite	± 3.0 m	7–8
KLX08-8	SKB 09713	451.62	Avrö granite	± 2.0 m	6–7
KLX08-9	SKB 09714	499.78	Avrö granite	± 16 m	6–7
KLX08-10	SKB 09715	550.23	Avrö granite	± 64 m	2–3
KLX08-11	SKB 09716	601.68	Diorite	± 2.3 m	3–4
KLX08-12	SKB 09717	660.03	Diorite	± 4.0 m	5–6
KLX08-13	SKB 09718	702.05	Diorite	± 23 m	7–8
KLX08-14	SKB 09719	750.80	Avrö granite	± 72 m	1–2
KLX08-15	SKB 09720	802.22	Avrö granite	± 52 m	1–2
KLX08-16	SKB 09721	857.98	Avrö granite	± 4.0 m	2–3
KLX08-17	SKB 09722	903.28	Avrö granite	± 47 m	2–3
KLX08-18	SKB 09723	945.75	Qtz-monzodiorite	± 92 m	5–6
KLX08-19	SKB 09724	983.18	Qtz-monzodiorite	± 17 m ²⁾	2–3

¹⁾ Approximate distance to next major alteration zone above and below sample.

²⁾ Minimum of 17 m since there are no data from below the maximum length of the borehole.

Table 2-3. Borehole KLX08: Experiments and measurements performed on drillcore samples.

Sample no	Water-content porosity	Density	Isotope diffusive exchange	Out-diffusion experiment Chemistry, pH, alkalinity	Sr and Cl isotopes	Chloride time-series
KLX08-1	X	X	O	X		X
KLX08-2	X	X	O	X		X
KLX08-3	X	X	X	X		X
KLX08-4	X	X	X	X	X	X
KLX08-5	X	X	X	X		X
KLX08-6	X	X	X	X	X	X
KLX08-7	X	X	X	X		X
KLX08-8	–	X	–	X		X
KLX08-9	X	X	–	X	X	X
KLX08-10	X	X	X	X	X	X
KLX08-11	X	X	X	X	X	X
KLX08-12	X	X	X	X		X
KLX08-13	X	X	X	X	X	X
KLX08-14	X	X	X	X	X	X
KLX08-15	X	X	X	X	X	X
KLX08-16	X	X	X	X		X
KLX08-17	X	X	X	X	X	X
KLX08-18	X	X	X	X		X
KLX08-19	X	X	X	X	X	X

X = Experiment performed, analyses available.

– = Inadequate material to perform the experiment.

O = Experiment performed, analytical data not produced based on final sample collection.

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. Unless otherwise stated, the analytics have been performed at this institution.

The water content was determined by the gravimetric determination of the water loss by drying drillcore subsamples at 105°C until stable weight conditions (± 0.002 g). If the material received allowed it, then the weight of these 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 water content was also determined on the material used for the isotope diffusive-exchange method using the same technique. These samples remained saturated throughout the experiment because they were placed in a vapour-tight vessel at 100% humidity during the equilibration procedure (see also below). The water-content porosity was calculated from the water loss and the volumetrically determined bulk wet density.

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 drillcore 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 stable water isotope composition of the pore water was determined by the isotope diffusive-exchange method as originally described by /Rogge 1997, Rübél 2000, Rübél et al. 2002/. 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 are stored together in a vapour-tight glass container. The mass and stable water isotope composition of the test water are known. In the test water about 0.3 mol NaCl are dissolved to lower the water vapour pressure above the test-water surface. This is to minimise loss of test water from the petri dish which would otherwise result in condensation on the rock fragments and the glass container walls. The petri dish with the test water and the whole container are weighed before and after the exchange experiment to check that no water is lost from the container and there was no transfer of test water to the sample by possible sorption on the rock material. Based on experience gained on samples from borehole KLX03, larger masses of rock were used in this experiment and equilibrium in the three reservoir system – rock sample, test water, and the air inside the container as a diaphragm – was achieved in about 20 to 30 days at room temperature depending on the size and water content of the rock pieces. After complete equilibration the test water was removed and analysed by ion-ratio mass spectrometry.

The isotope diffusive-exchange method 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 of borehole KLX08, the method was modified in that an artificial test water was used, which is strongly enriched in ^2H and depleted in ^{18}O ($\delta^{18}\text{O} = -109.84\%$ and $\delta^2\text{H} = + 425.5\%$ V-SMOW). In addition, smaller volumes of test water and larger masses of rock were used. These modifications were necessary in order to obtain a modified test water composition after equilibration that is outside the standard analytical error of the mass-spectrometer. Obviously, solutions so much enriched in ^2H are difficult to analyse for $\delta^2\text{H}$ and certain memory effects cannot be excluded for some of the samples. In contrast, the oxygen isotope data are more reliable.

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 drillcore samples of about 190 mm in height by immersion into the same artificial test water as used for the isotope diffusive-exchange method (Figure 2-1). 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. Weighing of the core before and after the experiment in addition gives valuable information about the saturation state of the core at the beginning of the experiment.

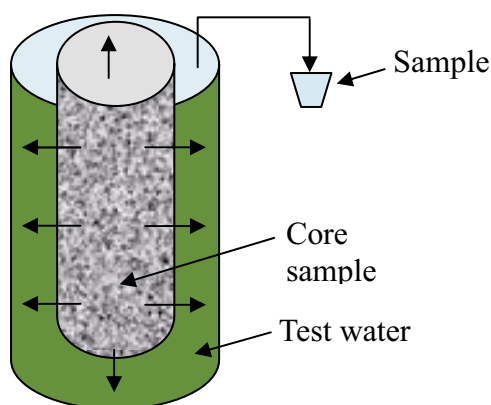


Figure 2-1. Schematic picture of out-diffusion experiments performed.

At specific time intervals, initially a few days and later a few weeks, 0.5 mL of solution were 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. The analytical error of these determinations is about 5% based on multiple measurements of the standard solutions.

After steady state with respect to chloride was achieved, 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 on a Metrohm 861 ion-chromatograph with a relative error of 5% based on multiple measurements of the standard solutions. Major cations and anions were analysed by ion-chromatography at Hydroisotop GmbH, Germany with a relative error of 5%.

The isotopic compositions of oxygen and hydrogen in the various test solutions (diffusive-exchange method, and out-diffusion experiments) were determined by conventional ion-ratio mass spectrometry at Hydroisotop GmbH. 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 $\delta^2\text{H}$.

The $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratio was measured at the University of Bern using a modified VG Sector[®] thermal ionisation mass spectrometer (TIMS) in simple collector mode, using oxidised Ta filaments. The analytical uncertainty is given with 2σ of multiple measurements of the same sample. Total Sr concentrations are given in ppm.

The $^{37}\text{C1}/^{35}\text{C1}$ isotopic ratio, expressed as $\delta^{37}\text{C1}$ relative to SMOC, was measured at the University of Waterloo Environmental Isotope Lab (EIL), Canada, using a VG SIRA 9 Mass Spectrometer. Measurements were made with a precision of $\pm 0.15\%$ (1σ) based on repeat analyses of SMOC.

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.

2.4 Nonconformities

The activity has been performed according to the activity plan without any significant nonconformities.

3 Tabulation of analytical data

Table 3-1. Water content by drying at 105°C, bulk density, and water-content porosity of rock samples from borehole KLX08.

Laboratory sample no	Lithology	Number of samples	Bulk density wet ¹⁾ (g/cm ³)	Water content average (wt.%)	Water content 1 σ (wt.%)	Water-content porosity average (vol.%)	Water-content porosity 1 σ (vol.%)
KLX08-1	Avrö granite	3	2.67	0.422	0.144	1.12	0.38
KLX08-2	Fine-grained granite	3	2.67	0.349	0.095	0.92	0.25
KLX08-3	Avrö granite	3	2.68	0.289	0.062	0.77	0.16
KLX08-4	Avrö granite	3	2.68	0.315	0.049	0.84	0.13
KLX08-5	Avrö granite	3	2.66	0.195	0.029	0.52	0.08
KLX08-6	Avrö granite	3	2.68	0.192	0.060	0.51	0.16
KLX08-7	Avrö granite	3	2.68	0.201	0.050	0.54	0.13
KLX08-8	Avrö granite	0 ²⁾	2.65	–	–	–	–
KLX08-9	Avrö granite	2	2.69	0.414	0.044	1.10	0.12
KLX08-10	Avrö granite	1	2.65	0.292	–	0.77	–
KLX08-11	Diorite	3	2.92	0.218	0.078	0.63	0.22
KLX08-12	Diorite	3	2.84	0.175	0.013	0.49	0.04
KLX08-13	Diorite	3	2.85	0.151	0.043	0.43	0.12
KLX08-14	Avrö granite	3	2.67	0.246	0.062	0.65	0.16
KLX08-15	Avrö granite	3	2.66	0.248	0.078	0.66	0.21
KLX08-16	Avrö granite	3	2.74	0.331	0.160	0.90	0.43
KLX08-17	Avrö granite	3	2.69	0.263	0.107	0.70	0.29
KLX08-18	Qtz-monzodiorite	3	2.81	0.183	0.080	0.51	0.22
KLX08-19	Qtz-monzodiorite	3	2.80	0.238	0.085	0.66	0.24

¹⁾ Determined from mass and volume of saturated (wet) drillcore sample used for out-diffusion experiment.

²⁾ Not enough sample material and/or fractured material received to perform analyses.

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

Laboratory sample no	Average depth along borehole (m)	$\delta^{18}\text{O}$ ¹⁾ pore water (‰ V-SMOW)	$\delta^2\text{H}$ ¹⁾ pore water (‰ V-SMOW)	Water content from isotope exchange (wt.%)	Water content error ^{1) 2)} 1σ (wt.%)
KLX08-1	150.22	–	–	–	–
KLX08-2	199.45	–	–	–	–
KLX08-3	200.26	–9.56	–83.5	<i>0.377</i>	<i>0.003</i>
KLX08-4	250.19	–8.58	–81.3	0.378	0.010
KLX08-5	302.34	–7.47	–76.7	0.183	0.003
KLX08-6	347.10	–8.58	–95.1	0.149	0.006
KLX08-7	395.65	–12.59	–105.6	0.258	0.003
KLX08-8	451.62	–	–	–	–
KLX08-9	499.78	–	–	–	–
KLX08-10	550.23	–13.99	–101.6	0.274	0.011
KLX08-11	601.68	–12.53	–100.8	0.137	0.009
KLX08-12	660.03	–8.50	–89.4	<i>0.452</i>	<i>0.007</i>
KLX08-13	702.05	–7.59	–83.9	0.187	0.007
KLX08-14	750.80	–5.15	–71.3	0.194	0.003
KLX08-15	802.22	–2.00	–54.4	0.159	0.007
KLX08-16	857.98	–9.72	–72.1	<i>0.725</i>	<i>0.004</i>
KLX08-17	903.28	–3.51	–53.1	0.189	0.007
KLX08-18	945.75	–6.89	–59.5	<i>0.366</i>	<i>0.003</i>
KLX08-19	983.18	–3.11	–43.0	0.233	0.007

¹⁾ Average error (calculated with Gauss' law of error propagation): $\delta^{18}\text{O} = \pm 1.7\text{‰}$, $\delta^2\text{H} = \pm 9.7\text{‰}$, and given for each sample for the water content.

²⁾ Rastered areas with data in italics: too high water content due to erroneous analysis of traced test water (memory effect during ^2H mass spectrometric measurement); pore-water $\delta^2\text{H}$ value remains unaffected within the error.

Table 3-3. Chemical composition of solutions from out-diffusion experiments at steady state conditions.

Out-diffusion experiment solution	Units	KLX08-1	KLX08-2	KLX08-3	KLX08-4	KLX08-5	KLX08-6	KLX08-7	KLX08-8
Sample description									
Depth along borehole	m	150.22	199.45	200.26	250.19	302.34	347.10	395.65	451.62
Rock type		Avrö granite	Fine-grained granite	Avrö granite	Avrö granite	Avrö granite	Avrö granite	Avrö granite	Avrö granite
Water-rock ratio		0.119	0.105	0.109	0.107	0.109	0.109	0.109	0.106
Experiment temperature	°C	45	45	45	45	45	45	45	45
Experiment time	days	91	91	91	91	91	91	91	93
Misc. properties									
Chemical type		$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$	$\frac{\text{Na}-\text{HCO}_3-\text{Cl}}{\text{Na}-\text{HCO}_3-\text{Cl}}$	$\frac{\text{Na}-\text{Ca}-\text{HCO}_3}{\text{Na}-\text{Ca}-\text{HCO}_3}$
pH (lab)	$-\log(\text{H}^+)$	7.64	7.74	7.51	7.42	7.5	7.18	7.21	7.47
Electrical conductivity	$\mu\text{S}/\text{cm}$								
Sample temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na^+)	mg/L	40.6	49.9	42.8	59.7	52.1	56.4	47.8	59.1
Potassium (K^+)	mg/L	3.2	4.2	3.0	2.7	2.1	4.0	1.1	3.4
Magnesium (Mg^{+2})	mg/L	1.6	2.8	2.0	1.2	0.5	1.3	0.1	0.2
Calcium (Ca^{+2})	mg/L	11.1	27.2	22.8	12.9	8.9	27.5	2	17.1
Strontium (Sr^{+2})	mg/L	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
Anions									
Fluoride (F^-)	mg/L	5.9	4.2	4.4	5.6	5.6	4.1	6.8	5.0
Chloride (Cl^-)	mg/L	3.4	4.5	4.3	3.4	12.5	13.5	6.7	6.4
Bromide (Br^-)	mg/L	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	<0.1	0.5
Sulphate (SO_4^{-2})	mg/L	2.8	4.6	3.2	5.5	5.8	5.3	6.9	5.1
Nitrate (NO_3^-)	mg/L	<0.5	<0.5	<0.5	4.2	1.5	<0.5	1.9	<0.5
Total alkalinity as HCO_3^-	mg/L	111.1	187.9	160.5	150.7	108.6	173.9	78.7	166.6
Calc. parameters									
Total dissolved solids	mg/L	178	283	241	241	196	285	150	263
Charge balance	%	5.16	4.63	3.04	5.66	4.33	6.29	4.83	3.59

Table 3-3. (Continued).

Out-diffusion experiment solution	Units	KLX08-9	KLX08-10	KLX08-11	KLX08-12	KLX08-13	KLX08-14	KLX08-15	KLX08-16
Sample description									
Vertical depth	m	499.78	550.23	601.68	660.03	702.05	750.80	802.22	857.98
Rock type		Avrö granite	Avrö granite	Diorite	Diorite	Diorite	Avrö granite	Avrö granite	Avrö granite
Water-rock ratio		0.101	0.106	0.096	0.113	0.099	0.110	0.108	0.106
Experiment temperature	°C	45	45	45	45	45	45	45	45
Experiment time	days	93	93	93	93	93	93	93	93
Misc. properties									
Chemical type		$\underline{\text{Na-Ca-HCO}_3\text{-Cl}}$	$\underline{\text{Na-Ca-HCO}_3\text{-Cl}}$	$\underline{\text{Na-Ca-HCO}_3}$	$\underline{\text{Na-Ca-HCO}_3}$	$\underline{\text{Na-Ca-HCO}_3}$	$\underline{\text{Na-Ca-HCO}_3\text{-SO}_4}$	$\underline{\text{Ca-NaSO}_4}$	$\underline{\text{Ca-Na-SO}_4}$
pH (lab)	-log(H ⁺)	7.24	7.47	7.32	7.13	7.37	7.14	7.01	7.01
Electrical conductivity	µS/cm								
Sample temperature	°C	20	20	20	20	20	20	20	20
Cations									
Sodium (Na ⁺)	mg/L	53.6	84.8	51.7	53.4	58.8	91.2	75.5	118.6
Potassium (K ⁺)	mg/L	3.4	3.1	6.4	7.8	8.1	6.0	10.7	17.2
Magnesium (Mg ⁺²)	mg/L	0.1	0.3	0.2	2.5	0.3	0.3	0.3	1.5
Calcium (Ca ⁺²)	mg/L	14.0	22.3	18.7	49.2	27.9	48.5	245.9	274.6
Strontium (Sr ⁺²)	mg/L	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	1.5	1.6
Anions									
Fluoride (F ⁻)	mg/L	4.8	4.0	3.6	3.2	1.1	4.0	2.4	2.0
Chloride (Cl ⁻)	mg/L	24.2	27.1	5.4	6.0	10.5	33.8	61.8	84.4
Bromide (Br ⁻)	mg/L	0.3	0.8	0.3	0.6	0.4	0.6	0.3	0.6
Sulphate (SO ₄ ⁻²)	mg/L	12.0	12.0	17.7	20.0	14.2	114.0	571.7	714.1
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	106.8	206.8	146.4	223.9	181.2	160.5	112.9	76.3
Calc. parameters									
Total dissolved solids	mg/L	219	360	250	366	302	458	1,081	1,289
Charge balance	%	3.08	2.92	3.73	7.83	7.23	3.12	0.74	2.21

Table 3-3. (Continued).

Out-diffusion experiment solution	Units	KLX08-17	KLX08-18	KLX08-19	Blank solution
Sample description					
Vertical depth	m	903.28	945.75	983.18	
Rock type		Avrö granite	Quartz-monzoniorite	Quartz-monzoniorite	
Water-rock ratio		0.108	0.104	0.105	
Experiment temperature	°C	45	45	45	
Experiment time	days	93	93	93	
Misc. properties					
Chemical type		Ca-Na-SO ₄	Na-Ca-HCO ₃ -Cl	Na-Ca-Cl-HCO ₃	
pH (lab)	-log(H ⁺)	6.98	7.27	7.47	
Electrical conductivity	µS/cm				14
Sample temperature	°C	20	20	20	20
Cations					
Sodium (Na ⁺)	mg/L	105.1	68.5	116.4	0.2
Potassium (K ⁺)	mg/L	14.0	10.7	10.4	<0.1
Magnesium (Mg ⁺²)	mg/L	0.4	0.5	0.7	0.3
Calcium (Ca ⁺²)	mg/L	241.9	48.1	68.8	0.1
Strontium (Sr ⁺²)	mg/L	0.9	<0.5	<0.5	
Anions					
Fluoride (F ⁻)	mg/L	2.1	2.4	3.1	<0.1
Chloride (Cl ⁻)	mg/L	145.4	53.4	183.1	1.1
Bromide (Br ⁻)	mg/L	1.2	1.0	1.8	<0.1
Sulphate (SO ₄ ⁻²)	mg/L	570.5	15.9	24.9	<0.1
Nitrate (NO ₃ ⁻)	mg/L	<0.5	0.0	1.1	
Total alkalinity as HCO ₃ ⁻	mg/L	60.4	195.3	153.2	<0.1
Calc. parameters					
Total dissolved solids	mg/L	1,140	394	560	<2
Charge balance	%	-0.12	4.82	2.49	2.57

Table 3-4. Isotopic composition of solutions from out-diffusion experiments at steady state conditions.

Laboratory sample no	Depth along borehole (m)	$\delta^{37}\text{Cl}$ ‰ V-SMOC	Sr ppm ²⁾	$^{87}\text{Sr}/^{86}\text{Sr}$	$^{87}\text{Sr}/^{86}\text{Sr}$ 1 σ
KLX08-1	150.22	–	–	–	–
KLX08-2	199.45	–	–	–	–
KLX08-3	200.26	–	–	–	–
KLX08-4	250.19	b.d. ¹⁾	0.185	0.715976	0.000013
KLX08-5	302.34	–	–	–	–
KLX08-6	347.10	b.d.	0.278	0.716791	0.000010
KLX08-7	395.65	–	–	–	–
KLX08-8	451.62	–	–	–	–
KLX08-9	499.78	0.4	0.190	0.717947	0.000032
KLX08-10	550.23	0.44	0.185	0.717305	0.000013
KLX08-11	601.68	b.d.	0.144	0.722642	0.000013
KLX08-12	660.03	–	–	–	–
KLX08-13	702.05	–	0.184	0.720575	0.000015
KLX08-14	750.80	3.43	0.492	0.715582	0.000011
KLX08-15	802.22	1.22	1.320	0.714670	0.000010
KLX08-16	857.98	–	–	–	–
KLX08-17	903.28	1.26	2.042	0.713231	0.000019
KLX08-18	945.75	–	–	–	–
KLX08-19	983.18	0.66	0.856	0.715639	0.000016

¹⁾ b.d. = below detection due to low Cl content. ²⁾ Mass-spectrometric measurement.

Table 3-5. Chloride concentration of pore water calculated from out-diffusion solutions and the water content of the samples.

Laboratory sample no	Depth along borehole (m)	Lithology	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)
KLX08-1	150.22	Avrö granite	99	24	49
KLX08-2	199.45	Fine-grained granite	139	29	50
KLX08-3	200.26	Avrö granite	164	28	44
KLX08-4	250.19	Avrö granite	117	15	21
KLX08-5	302.34	Avrö granite	705	90	122
KLX08-6	347.10	Avrö granite	773	180	341
KLX08-7	395.65	Avrö granite	365	71	118
KLX08-8	451.62	Avrö granite	–	–	–
KLX08-9	499.78	Avrö granite	614	56	69
KLX08-10	550.23	Avrö granite	998	100	100
KLX08-11	601.68	Diorite	240	61	129
KLX08-12	660.03	Diorite	388	27	31
KLX08-13	702.05	Diorite	687	150	270
KLX08-14	750.80	Avrö granite	1,534	302	506
KLX08-15	802.22	Avrö granite	2,722	637	1,221
KLX08-16	857.98	Avrö granite	2,764	873	2,504
KLX08-17	903.28	Avrö granite	6,059	1,709	4,048
KLX08-18	945.75	Qtz-monzodiorite	3,041	909	2,319
KLX08-19	983.18	Qtz-monzodiorite	8,228	2,112	4,448

¹⁾ Error based on the standard deviation of multiple water-content measurements

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