

**Methodology for hydrogeochemical sampling to characterise
groundwaters in crystalline bedrock: developments made within
the Swedish radwaste programme. Supplementary Material**

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Supplementary Material 1: **Background**

The need for reliable groundwater sampling procedures and chemical analyses has been internationally recognised for years. The USGS (United States Geological Survey) was one of the first institutions in the 1970s to publish rigorous sampling and analytical protocols and procedures related to studies of environmental groundwater contamination ([1], although the first edition was published in 1959; [2, 3]). Since then, and together with USEPA (United States Environmental Protection Agency), more detailed descriptions, proposals and manuals of sampling procedures, devices, techniques, etc. in different host rocks, have been reported in various publications by these two organisations [4-14]. Along similar lines, other countries such as Australia and South Africa have recently published guidelines for groundwater sampling [15, 16] which are based on previous experience developed since 1997, involving drilling, sampling, analytical methodologies and quality assessment [17-20].

There are many other domains in which the deep drilling and the related investigations have also evolved and improved over the years (geothermalism, ODP, etc) but in this summary we will focus on the context of radioactive waste disposal. In this context, most of the existing technologies for sampling in boreholes to around 1,000 m depth have been developed and documented in several international site characterisation projects. Furthermore, natural analogue studies have also provided valuable input in this respect (e.g. [21-22]). Overall, it is important to stress that collaboration between these international organisations has been close, particularly where similar rock types have been demarcated for radioactive waste disposal; some notable examples are briefly listed below.

Site investigations carried out by AECL (Atomic Energy of Canada Ltd.) and now by NWMO, (the Nuclear Waste Management Organization) on the Canadian Shield commenced in 1978 and resulted in important developments of borehole and sampling techniques for hydrogeochemical investigations in fractured crystalline rocks [5, 23-33].

In Switzerland, a major effort has been made since the 1980's by NAGRA (National Cooperative for the Disposal of Radioactive Waste) on drilling and development of characterisation methodologies related to deep boreholes initially in crystalline rocks [34-44] and more recently in clay formations [40].

The Finnish site investigation programme carried out initially by TVO (Teollisuuden Voima Oyj) and later by Posiva Oy, started in 1984 and was mainly focused on groundwater flow and geochemistry due to their importance in terms of long-term repository safety in crystalline rock. These studies resulted in, for example, the development of field instrumentation and tests and protocols for groundwater sampling and measuring groundwater flow [45-58]. Also included were analytical programmes which covered, for example evaluation of the representativeness of the groundwater samples, use of sampling equipment, and handling and preparation of groundwater samples, as well as field measurements and analyses.

In Spain, the main scientific and technological advance on the hydrogeochemical investigations for deep geological disposal started with ENRESA (Empresa Nacional de Residuos Radioactivos, SA) in 1984. Then, in the 1990s a specific and comprehensive protocol for the groundwater sampling and characterisation was developed in the framework of the International Natural Analogue Project at El Berrocal [59-63].

In Belgium and France, where radioactive wastes disposal in clay repositories are being considered by ONDRAF/NIRAS (Organisme National des Déchets RAdiactifs et des matières Fissiles enrichies) and ANDRA (Agence Nationale pour la gestion des Déchets RAdioactifs), technological and methodological developments have been carried out in relation to the hydrogeochemical characterisation of underground research laboratories in clay [64-67].

In the United Kingdom the first publications concerning deep borehole sampling, sample handling and storage and chemical analyses were associated with the Sellafield site investigations [68-73]. More recently the NDA-RWMD (Nuclear Decommissioning Authority - Radioactive Waste Management Directorate) have published several reports related to groundwater sampling and analytical strategies and techniques as part of a future site characterisation programme for a geological

radioactive waste disposal facility [74-79]. The work from Bath and Metcalfe [75] provides a thorough review of the available technologies for groundwater sampling and analyses developed in site characterisation projects on three relevant host rock types. The authors give a general overview of the sampling methods and techniques, the operational information about the equipment and information about the countries that have developed the equipment (Tables 5-1, 5-2, 5-5 and 6-1 in [75]). They also discuss the quality of groundwaters in terms of their representativity. The United Kingdom programme has still not been restricted to any specific rock type.

The Japanese hydrogeochemical investigations related to the deep geological disposal of radioactive wastes started in the 1990s and were carried out by the JNC (Japan Nuclear Cycle Development Institute). Some specific methodologies have been developed [80-81] and others have been applied based on experience from other countries. All these developments were initially studied in the Kamaishi and Tono Mines [82-86] and, more recently in the Mizunami and Horonobe Underground Research Laboratories [87-95]. This experience has been incorporated in the procedures that constitute the scientific and technical basis for HLW (High Level Wastes) disposal in Japan [96-100].

Sweden (through the Swedish Nuclear Fuel and Waste Management Company, SKB) together with Finland, has had the advantage of a continuous programme of scientific and technical development of a site characterisation for almost 40 years. Since 1977 SKB has performed activities with the overall objective of acquiring knowledge and data to develop methodologies and instrumentation required for the safe disposal of radioactive wastes in fractured crystalline rocks. An important part of this work has been the hydrogeochemical characterisation of the deep groundwaters in granitic rocks, in order to describe their chemistry, origin and distribution in the bedrock and the hydrogeochemical processes involved in their evolution. Close collaboration with other agencies, such as those listed above, has been a great benefit in this respect.

The Swedish site characterisation programme initially investigated a number of crystalline rock sites with the aim to increase knowledge of bedrock conditions in different types of rocks and at different locations in Sweden (SKB Study Site Programme; 1976-2001). Together with these investigations, a

final repository for low- and intermediate-level radioactive waste (SFR), located adjacent to Forsmark at the Baltic coast about 150 km north of Stockholm, commenced operations in 1988.

At the time of these early Study Site investigations (1976-1986) very little was known about the groundwater chemistry at 500 m depth in non-mineralised crystalline bedrock and therefore a progressive development of a specific investigation methodology was initiated. The initial reports on sampling and analysis protocols for groundwaters were published by SKB at the beginning of the 1980s associated with the establishment of the KBS-3 disposal concept [101-103], and the characterisation of several sites [104-112]. High quality groundwater data was already recognised at that time as a necessary pre-requisite in site characterisation and, therefore, evaluation of the quality of groundwater samples was an important part of the studies [113-116]. Due to the complexity of the fracture systems, these studies showed the lack of representative groundwater samples for hydrochemical considerations [113] and, therefore, an important effort was made to rectify this. It involved improving instrumental development, experimenting using different materials, testing drilling and sampling techniques and analysing their effects on the final chemical composition of the sampled groundwaters. These successful experiments and associated knowledge subsequently became an integrated part of the SKB approach.

One of the major improvements was the design and use of the first mobile chemistry equipment in 1984. It included a mobile laboratory for immediate chemical analyses and down-hole equipment for, among other uses, to carry out *in situ* Eh and pH measurements. This new methodology regarding redox measurements was of special relevance since the general belief at the time was that it was not possible to measure meaningful Eh values in natural waters.

However, despite the important advances made thanks to this mobile equipment, some problems still remained, for example it was not realised how difficult it was to obtain representative groundwater samples; another problem was the lack of good analytical methods for isotope determinations (especially for ^{14}C and ^3H) which prevented the reliable use of these isotopes for residence time interpretations.

Prior to the construction of the Äspö Hard Rock Laboratory (1986-1990), the *pre-investigation* studies represented important progress from the earlier KBS-3 groundwater studies in refining and establishing future borehole investigation methodology [117-118]. A major step forward was the introduction of a new drilling technique, telescope-type drilling, which improved the possibilities to remove flushing water and drilling debris, thereby increasing the quality of the groundwater samples. The investigations in boreholes from the Äspö tunnel during the following *construction phase* (1990-1995; [119-120]) were performed in parallel with the construction work which required careful planning. The *operation phase* in the late 1990s involved the introduction of differential flow logging measurements [49, 121] and BIPS logging measurements (Borehole Image Processing System; [122]) techniques which significantly improved the possibility of selecting water bearing fractures for sampling and determining the water yield situation in demarcated borehole sections. Furthermore, the tripple tube drilling system minimised the loss of fracture filling material therefore improving the quality of the fracture mineral samples, which are very important for the hydrogeochemical interpretations from several aspects. During this time much effort was also spent on the thorough assessment of all procedures involved in the localisation, sampling and analysis of groundwaters to find sources of uncertainties or inconsistencies in the final groundwater chemical data. Laaksoharju et al. [123], Smellie et al. [124] and Laaksoharju [125] describe in detail different quality evaluation approaches (expert judgement, statistical treatment and scoring system) used to identify representative chemical compositions for classification and modelling purposes.

Based on this experience gained over a period of about 20 years, SKB published a series of documents outlining the basis for the geoscientific programme for investigation and evaluation of sites for a deep repository ([126] and references therein). The general investigation programme was established in SKB [127] and the guidelines and strategy for the hydrogeochemical interpretation and modelling work were described in detail in Smellie et al. [128]). However, the details about the groundwater sampling issues were not addressed in any of these previous publications.

During the site characterisation investigations at Forsmark, Laxemar and SFR (2002 to 2010; 4-6) to select the location for the final repository of spent nuclear fuel (the two first) and for the extension of

the existing repository (SFR) for low and intermediate level waste, a large number of boreholes were drilled and newly developed or modified hydrochemical investigation methods were applied for studying the groundwater chemistry [129-132]. Although these investigations were planned based on the previous experience, modifications, updates and improvements on the methodologies and strategies had to be done and they are presented and discussed in this paper. SKB will use the same kind of methodological scheme during repository construction and operation with modifications and future technical developments. Additional publications concerning specific SKB methodologies related to the hydrogeochemical studies have been published and will not be described in detail here, e.g. the methodology developed for potentiometrical Eh measurements and their evaluation [133], the methodology used for the matrix porewater studies [134, 135], the studies on microbes and gases [136, 137], on fracture minerals [138-143], and on statistical and hydrogeochemical modelling techniques [144, 145].

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Supplementary Material 2: **Drilling and after drilling procedures**

This file contains some detailed description on different steps of the drilling and after drilling procedures (see Figure 1 in the main paper), including the issues about the flushing water and the cleaning, that complement the summary included in the main paper.

SM2.1 THE FLUSHING WATER

One of the most important aspects when evaluating groundwater samples and groundwater data from core boreholes drilled from the ground surface is the degree of contamination with flushing water and its impact on the groundwater chemistry and sample representativity. Typically, about 1,000 m³ flushing water (spiked with sodium fluorescein as tracer) is used for a 1,000 m long SKB type telescopic core borehole drilled from the ground surface. About twice this volume (2,000 m³) is discharged (depending on water yield) from a borehole during gas-lift pumping from the uppermost 100 m of the borehole at a flow rate between 20 and 50 L/min. The gas-lift pumping removes the return water, i.e. a mixture of flushing water, groundwater and drill cuttings, from the borehole.

The risk of flushing water contamination is much lower in samples collected from boreholes drilled in underground tunnels since the flow direction is out from the borehole due to the hydrostatic overpressure. However, special conditions may arise where contamination is difficult to avoid, for example if two boreholes are hydraulically connected or if there is a hydraulic gradient along the borehole.

In any case, due to contamination risks, the choice of a flushing water source is very important. Two possible strategies are used: 1) flushing water with a chemical composition similar to the groundwater expected to be found in the borehole to minimise the influence on the samples, i.e. flushing water taken from an adjacent percussion borehole, implicitly assuming that the composition will be quite

close, or 2) tap water with much lower concentrations of most components and therefore not likely to affect the interpretation of the groundwater origin (e.g. marine or non-marine signatures). The first alternative has been the most common choice but its main disadvantage is that the groundwater composition is unknown beforehand, and it varies with depth. Consequently, the composition of the flushing water and the groundwater in the borehole being drilled may differ considerably. The second alternative, on the other hand, results in dilution of the groundwater sample. This dilution is usually manageable when interpreting the data. However, parameters such as TOC/DOC may be significantly higher in the tap water and can therefore obstruct the evaluation of the organic component in the formation water. The tap water contribution is also a problem when analysing ^{14}C in organic material and in inorganic carbon.

Another important aspect when selecting the flushing water source is the probable effect of its oxygen content on the groundwater redox conditions. Therefore, nitrogen gas is bubbled into the flushing water (irrespective of its source) before use (cf. Figure SM2.1). An estimation of the impact of the flushing water on the groundwater composition is always carried out during the data interpretation process. A flushing water budget is calculated [146] for each drilled borehole.

With respect to the cleaning, for hydrochemical and microbial investigations the specialised SKB telescopic borehole requires a strict routine of cleanliness and sterility. The down-hole equipment and the flushing water system (see below) undergo rigorous cleaning procedures: 1) the pipe string and drilling crown are steam cleaned before use, 2) the drilling water supply tube line is cleaned and scanned using UV-light for sterilisation (Figure 2), and 3) the bioaccessibility of all the used chemical products are also thoroughly addressed including the choice of lubricants for connecting the pipe string. However, despite these precautions, it would be unrealistic to expect total sterile conditions.

SM2.2. AFTER DRILLING

After drilling (see Figure 1 in the main manuscript), the boreholes are usually cleared of rock debris and drilling water by gas-lift pumping (N_2). The detailed core mapping activity starts as soon as the drill core is removed and transported to the core mapping hall/facility. Hydrochemical logging (tube sampling) is performed relatively early in the investigation sequence with the purpose of obtaining the

composition of the groundwater present along the borehole. Also obtained early in the sequence are data from the different geophysical logging methods which are needed to proceed with the ongoing core mapping activity. The same applies to the differential flow logging which is used, together with the information from the BIPS logging (Borehole Image Processing System), to select the water yielding fracture(s) to be hydrochemically characterised and to isolate suitable borehole sections to be investigated. Extensive hydrochemical characterisation (Complete Chemical Characterisation or CCC) implies investigations in one packed-off borehole section at a time, and most often it also includes colloid, gas and microbial studies.

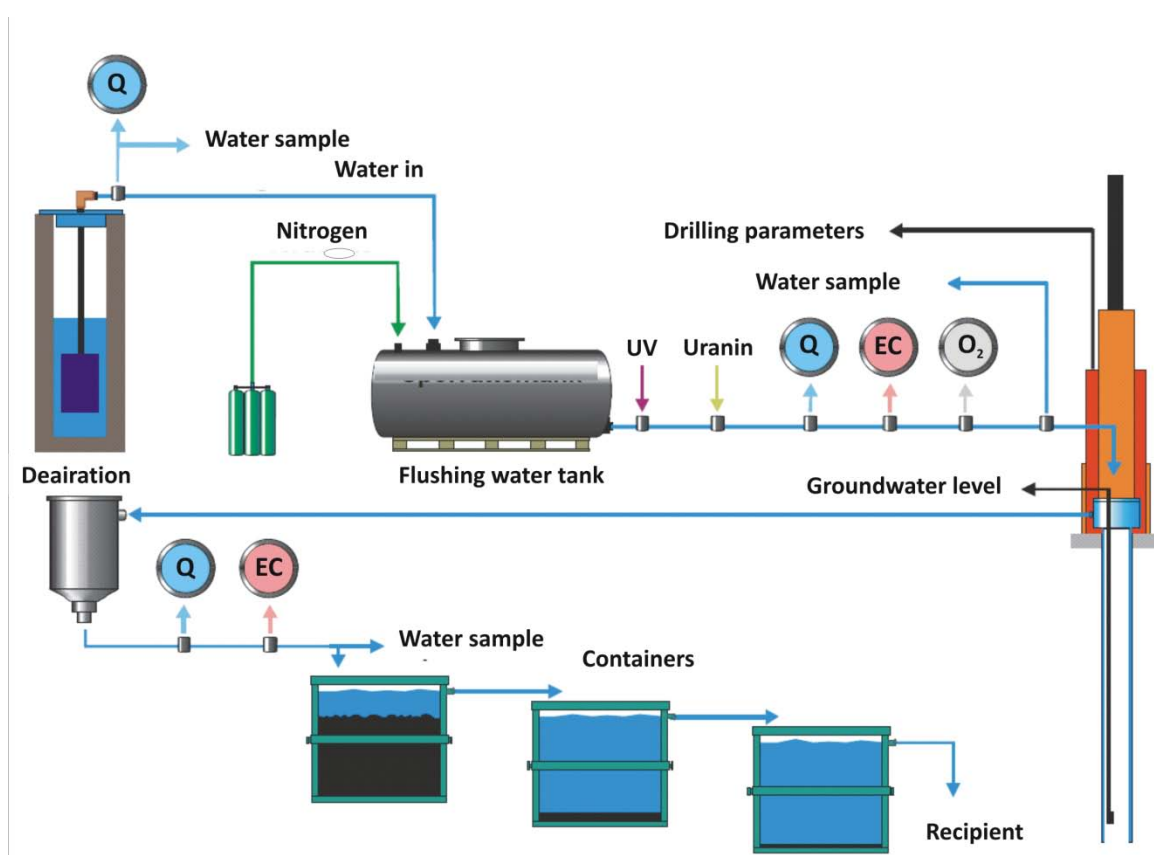


Figure SM2.1. Schematic outline of the flushing water line and the treatment of returned water. The different measurement stations and sampling points are also displayed (modified from drilling method description SKB MD 640.001) UV = Ultra Violet light used for sterilisation, Uranine = injection location for uranine (sodium fluoresceine; the flushing water is spiked with uranine as tracer), Q = water flow rate measurement, EC = Electrical Conductivity measurement, O₂= dissolved oxygen measurement. Figure courtesy of Göran Nilsson.

Once the main hydrochemical characterisation campaign has finished, other more extensive hydraulic tests are performed that are likely to contaminate the groundwater; these include injection and interference tests and groundwater flow measurements. These are not performed until any pressure disturbances caused by water sampling have disappeared, i.e. if water sampling has been carried out for two weeks, then the hydraulic tests are postponed for at least another two weeks after the water sampling.

When the above basic investigation activities have finished, fixed packer equipment is installed to prevent groundwater flow along the borehole and ultimately to allow regular groundwater level monitoring, sampling and flow measurements in the packed-off borehole sections. Thereafter, hydrochemical monitoring is performed in selected borehole sections (i.e. regular yearly sampling; [147]).

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Supplementary Material 3: **Supplementary Tables**

This file includes two tables that give detailed information on some of the methodological aspects treated in the paper, specifically in Sections 4.1 and 5.3. Table SM3-1 lists the analytical protocol followed for the groundwaters, including the detection limits and the measurement uncertainties. Table SM3-2 displays an example of cornerstone criteria that were found to be relevant independently of the type of dataset.

Table SM3-1. List of components usually analysed in the hydrochemical investigations. Many elements may be determined by more than one ICP technique depending on concentration range. The most relevant technique and measurement uncertainty for the concentrations normally encountered in groundwater are indicated. In cases where two techniques were frequently used, both are displayed under the Method column. The analyses generally follow the standards from the Swedish Standards Institute (SIS) and Comité Européen de Normalisation (EN) or the US Environmental Protection Agency (USEPA). Reporting limits (RL) are generally 10×standard deviation. Measured values below RL or DL are stored as negative values in SICADA (i.e. –RL value and –DL value). The reporting limits are given if not otherwise stated. Measurement uncertainty reported by the laboratory is generally as ±percent of measured value in question at 95% confidence interval, calculated according to the EURACHEM/CITAC guide (2000).

Component	Method*	Reporting limits (RL), detection limits (DL) or range	Units	Measurement uncertainty
pH	Potentiometric	3-10	pH unit	±0.1
EC	Conductivity meter	1-150 150-10,000	mS/m	5% 3%
HCO ₃	Alkalinity titration	1	mg/L	4%
Cl ⁻	Mohr- titration	≥ 70	mg/L	5%
Cl ⁻	IC	0.5 – 70	mg/L	8%
SO ₄	IC	0.5	mg/L	12%
Br ⁻	IC	DL 0.2, RL 0.5	mg/L	15%
Br	ICP SFMS	0.001, 0.004, 0.010 ¹	mg/L	25% ²
F ⁻	IC	DL 0.2, RL 0.5	mg/L	13%
F ⁻	ISE	DL 0.1, RL 0.2	mg/L	12%
I ⁻	ICP SFMS	0.001, 0.004, 0.010 ¹	mg/L	25% ²
Na	ICP AES	0.1	mg/L	13%
K	ICP AES	0.4	mg/L	12%
Ca	ICP AES	0.1	mg/L	12%
Mg	ICP AES	0.09	mg/L	12%
S(tot)	ICP AES	0.16	mg/L	12%
Si(tot)	ICP AES	0.03	mg/L	14%
Sr	ICP AES	0.002	mg/L	12%
Li	ICP AES	0.004	mg/L	12.2%
Fe	ICP AES	0.02	mg/L	13.3% ³
Fe	ICP SFMS	0.0004, 0.002, 0.004 ¹	mg/L	20% ³
Mn	ICP AES	0.003	mg/L	12.1% ²
Mn	ICP SFMS	0.00003, 0.00004, 0.0001 ¹	mg/L	53% ³
Fe(II), Fe(tot)	Spectrophotometry	DL 0.006, RL 0.02	mg/L	0.005 (0.02-0.05 mg/L) 9% (0.05-1 mg/L) 7% (1-3 mg/L)
HS-	Spectrophotometry, SKB	SKB DL 0.006, RL 0.02	mg/L	30%
HS-	Spectrophotometry, external laboratory	0.01	mg/L	0.02 (0.01-0.2 mg/L) 12% (>0.2 mg/L)
NO ₂ as N	Spectrophotometry	0.1	µg/L	2%
NO ₃ as N	Spectrophotometry	0.2	µg/L	5%
NO ₂ +NO ₃ as N	Spectrophotometry	0.2	µg/L	0.2 (0.2-20 µg/L) 2% (> 20 µg/L)
NH ₄ as N	Spectrophotometry, SKB	11	µg/L	30% (11-20 µg/L) 25% (20-50 µg/L) 12% (50-1200 µg/L)
	Spectrophotometry external laboratory	0.8	µg/L	0.8 (0.8-20 µg/L) 5% (> 20 µg/L)
PO ₄ as P	Spectrophotometry	0.7	µg/L	0.7 (0.7-20 µg/L) 3% (> 20 µg/L)
SiO ₄	Spectrophotometry	1	µg/L	2.5% (>100 µg/L)
O ₂	Iodometric titration	0.2 – 20	mg/L	5%

Table SM3-1. Continuation.

Component	Method	Reporting limits (RL), detection limits (DL) or range	Units	Measurement uncertainty
O ₂	Iodometric titration	0.2 – 20	mg/L	5%
Al,	ICP SFMS	0.2, 0.3, 0.7 ¹	µg/L	17.6% ³
Zn	ICP SFMS	0.2, 0.8, 2 ¹	µg/L	15.5, 17.7, 25.5% ³
Ba, Cr, Mo,	ICP SFMS	0.01, 0.04, 0.1 ¹	µg/L	Ba 15% ¹ , Cr 22% ² Mo 39% ³
Pb	ICP SFMS	0.01, 0.1, 0.3 ¹	µg/L	15% ³
Cd	ICP SFMS	0.002, 0.02, 0.5 ¹	µg/L	15.5% ³
Hg	ICP AFS	0.002	µg/L	10.7% ³
Co	ICP SFMS	0.005, 0.02, 0.05 ¹	µg/L	25.9% ³
V	ICP SFMS	0.005, 0.03, 0.05 ¹	µg/L	18.1% ³
Cu	ICP SFMS	0.1, 0.2, 0.5 ¹	µg/L	14.4% ³
Ni	ICP SFMS	0.05, 0.2, 0.5 ¹	µg/L	15.8% ³
P	ICP SFMS	1, 5, 40 ¹	µg/L	16.3% ³
As	ICP SFMS	0.01 (520 mS/m)	µg/L	59.2% ³
La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu	ICP SFMS	0.005, 0.02, 0.05 ¹	µg/L	20%, 20%, 25% ³
Sc, In, Th	ICP SFMS	0.05, 0.2, 0.5 ¹	µg/L	25% ³
Rb, Zr, Sb, Cs	ICP SFMS	0.025, 0.1, 0.25 ¹	µg/L	15%, 20%, 20% ² 25% ³
Tl	ICP SFMS	0.025, 0.1, 0.25 ¹	µg/L	14.3% ^{2 and 3}
Y, Hf	ICP SFMS	0.005, 0.02, 0.05 ¹	µg/L	15%, 20%, 20% ² 25% ³
U	ICP SFMS	0.001, 0.005, 0.01 ¹	µg/L	13.5%, 14.3%, 15.9% ² 19.1%, 17.9%, 20.9% ³
DOC	UV oxidation, IR detection Carbon analysator	0.5	mg/L	8%
TOC	UV oxidation, IR detection Carbon analysator	0.5	mg/L	10%
δ ² H	MS	2	‰ SMOW ⁴	0.9 (one standard deviation)
δ ¹⁸ O	MS	0.1	‰ SMOW ⁴	0.1 (one standard dev.)
³ H	LSC	0.8	TU ⁵	0.8
δ ³⁷ Cl	AMS	0.2	‰ SMOC ⁶	0.2 ¹²
δ ¹³ C	AMS	-	‰ PDB ⁷	0.3 ¹²
¹⁴ C pmc	AMS	-	PMC ⁸	0.4 ¹²
δ ³⁴ S	MS	0.2	‰ CDT ⁹	0.4 (one standard dev.)
⁸⁷ Sr/ ⁸⁶ Sr	TIMS	-	No unit (ratio) ¹⁰	0.00002
¹⁰ B/ ¹¹ B	ICP SFMS	-	No unit (ratio) ¹⁰	-
²³⁴ U, ²³⁵ U, ²³⁸ U, ²³² Th, ²³⁰ Th	Alfa spectr.	0.0001	Bq/L ¹¹	≤5% (Counting statistics uncertainty)
²²² Rn, ²²⁶ Ra	LSC	0.015	Bq/L	≤5% (Counting statistics uncertainty)

* Analytical methods abbreviations:

AMS: Accelerator Mass Spectrometry

IC: Ion Chromatography

ICP-AES: Inductively Coupled Plasma Atomic Emission Spectrometry

ICP-AFS: Inductively Coupled Plasma Atomic Fluorescence Spectrometry

ICP-SFMS: Inductively Coupled Plasma Sector Field Mass Spectrometry

ISE: Ion Selective Electrode

LSC: Liquid Scintillation Counting

MS: Mass Spectrometry

TIMS: Thermal Ionisation Mass Spectrometry

Table SM3-1. Continuation.

1. Reporting limits at electrical conductivity 520 mS/m, 1440 mS/m and 3810 mS/m respectively.
2. Measurement uncertainty at concentrations 100×RL
3. Measurement uncertainty at concentrations 10×RL
4. Per mille deviation from SMOW (Standard Mean Oceanic Water). Isotopes are often reported as per mill deviation from a standard. The deviation is calculated as: $\delta^i = 1000 \times (K_{\text{sample}} - K_{\text{standard}}) / K_{\text{standard}}$, where K= the isotope ratio and $^i = {}^2\text{H}$, ^{18}O , ^{37}Cl , ^{13}C or ^{34}S etc.
5. TU=Tritium Units, where one TU corresponds to a tritium/hydrogen ratio of 10⁻¹⁸ (1 Bq/L Tritium = 8.45 TU).
6. Per mille deviation from SMOC (Standard Mean Oceanic Chloride).
7. Per mille deviation from PDB (the standard PeeDee Belemnite).
8. The following relation is valid between pmC (percent modern carbon) and Carbon-14 age: $\text{pmC} = 100 \times e^{((1950-y) \cdot 1.031/8274)}$ where y = the year of the C-14 measurement and t = C-14 age.
9. Per mille deviation from CDT (the standard Canyon Diablo Troilite).
10. Isotope ratio without unit.
11. The following expressions are applicable to convert activity to concentration; for uranium-238 and thorium-232: 1 ppm U = 12.4 Bq/kg ²³⁸U, 1 ppm Th = 3.93 Bq/kg ²³²Th.
12. SKB estimation from duplicate analyses by the contracted laboratory.

Table SM3-2. An example of a criteria table with category grading. Each criterion has its grade and the final category grading for the sample is determined by the worst grade/highest number. The table presented here is derived from similar tables developed during past SKB site investigations (Table 3-2 in [148]; Table 4-1 in [149]; Table 3-2 in [150]; and Table A1-1 in [151]). These categorisation criteria should be adapted to the conditions of the specific conditions for each site investigation.

Criteria	Category grade				
	1	2	3	4	5
Drill water					
(<2 %)	X				
(<5 %)		X			
(<10 %)			X		
(>10 %)					X
Sampling method					
Sampling during drilling					X
Sampling in an isolated section in a surface (CCC) or in a tunnel borehole	X				
Monitoring in fixed borehole sections in surface boreholes				X	
Monitoring in fixed borehole sections in tunnel boreholes	X				
Available data (major constituents and basic components with lower concentrations)					
Complete major constituents (Na, K, Ca, Mg, Cl, HCO ₃ ⁻ , SO ₄ ²⁻) and ions with lower concentration (Si, Br, Sr, Li, F, S(II) Fe, Mn).	X				
Ions with lower concentrations are incomplete: one or more of them are missing.		X			
Uncertain pH-value			X		
One of the following components are missing: K, Mg, HCO ₃ , or SO ₄ .				X	
The major constituents are incomplete: more than one of them are missing.					X
Charge imbalance					
>±5% (±10% at <50 mg/L Cl)					X
Available isotope data					
Complete: δ ¹⁸ O, δ ² H, ³ H, ¹⁴ C, δ ¹³ C (except in samples with HCO ₃ < 10 mg/L)	X				
δ ¹⁸ O, δ ² H, ³ H		X			
δ ¹⁸ O, δ ² H			X		
Incomplete: lack of δ ¹⁸ O and/or δ ² H				X	
Section length					
(<10 m)	X				
(<20 m)		X			
(<100 m)			X		
(>100 m)				X	
Sample series*					
Adequate number of samples (to follow the development during months- years)	X				
Inadequate number of samples			X		
Time series**:					
Adequate number of samples (at least three samples during days-weeks).	X				
One or two samples				X	
Significant impact from injection of grout (enhanced pH value)					X

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Note: the following reports may be downloaded from <http://www.skb.com/publications/>

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