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Compositions of groundwater for SFR and its extension, during different climate cases, SR-PSU

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Abstract

This study was performed to support the assessment of long-term safety for the final repository for low- and intermediate-level radioactive waste (SR-PSU) at Forsmark, SFR. The SR-PSU safety assessment is an important document to be included in the license application for the existing SFR 1 and planned extension SFR 3, which is being prepared by the Swedish Nuclear Fuel and Waste Management Company (SKB 2014). One of the questions to be addressed as part of this application is whether the hydrogeochemical environment around the repository will remain favourable for the stability of the wastes and the retention of the radionuclides over time during the expected climatic environmental evolution.

Many of the variables that may affect the repository perfomance are directly or indirectly affected by the chemical composition of the groundwater in the rock volume surrounding the repository. Moreover, different groundwater compositions will prevail as a result of the different types of climate domains and their corresponding hydraulic conditions and the succession of these periods will affect the flow and the composition of the groundwater around the repository.

The study presented in this report discusses and describes the estimation of the reference groundwater compositions around the repository for different climatic conditions. The future climate evolution in Forsmark is represented by a range of four climate cases in SR-PSU. The evolution of climate conditions in each climate case is represented by a succession of so called climate domains. The discussion about the future evolution of the chemical groundwater composition is based on reference groundwater compositions estimated to prevail around the repository in the three different climate domains: temperate, periglacial and glacial.

Two possible situations have been addressed for the *temperate periods*: 1) site covered by the Baltic Sea (as today) and 2) site emerged above the sea level due to isostatic uplift. In the first case, the proposed water composition corresponds to brackish-saline groundwater (similar to the situation at present), whereas in the second case land uplift will allow the input of fresh (non-saline) groundwater from the recharge inland areas into the repository.

The sparse information available indicates that the effect of permafrost conditions on the groundwater hydrochemistry is negligible. Based on the presently available information, the groundwaters expected to be around the repository periods of *periglacial climate domain* will be similar to the waters considered for the temperate domain both in the case of submerged and emerged conditions.

Finally, in periods of *glacial climate domain* the repository will be located beneath an ice sheet and inflowing ice meltwater of low salinity will saturate the repository. The proposed composition of this water is based on data from the Swedish Site Investigations and on the hydrochemical review of the glacial-derived groundwaters found in those investigations.

The selection of the reference groundwater composition for each climate domain and submerged/emerged conditions was based on chemical analyses, compilations, reviews and conclusions available from the Site Characterisation Programmes of Forsmark, Laxemar and the SFR. In some cases, additional datasets (e.g. from wells, experiments, monitoring programmes and other sampling campaigns in Forsmark, Laxemar and SFR, or from regional data in northern Uppland) have been included for comparison.

The main objective of this study was to estimate reference groundwater compositions around the SFR repository in Forsmark in periods of different climate domains, and submerged/emerged conditions. The impact of extended periods of a specific climate domain and shorelevel conditions is also assessed. The resulting reference groundwater compositions will be used in different modelling activities within the SR-PSU safety assessment.

Contents

1 Introduction

1.1 Background

The Swedish Nuclear Fuel and Waste Management Company (SKB) has a plan for a future extension of the final repository for short-lived low and intermediate level radioactive operational waste, SFR, located about 150 km north of Stockholm. The purpose is to select a bedrock volume large enough to allow further storage of operational waste from existing Swedish nuclear power plants and future waste from the decommissioning and dismantling of nuclear power plant reactors (SKB 2008a). Of several alternatives, a selected location was investigated southwest of the present SFR tunnel system (Figure 1-1). It is intended that the new storage capacity will connect with the existing SFR facility (at –117 m in the bedrock under the Baltic Sea) and thus the target area for the location of the extension is already defined.

In order to characterise the selected location a Site Descriptive Model of the SFR site (SDM-PSU; SKB 2013a) was produced based on the integrated understanding of the historic data acquired from the investigations for the construction of the existing SFR facility (year 1980–1986), as well as, from the recent investigations for the planned extension of SFR (year 2008–2009). The SDM-PSU is an integrated model for geology, hydrogeology and hydrogeochemistry, including also a description of the surface system and a summary of the abundant underlying data and the discipline-specific models that support the site understanding.

In the assessment of long term safety for the SFR repository (SKB 2014), a probable future evolution of importance for the long-term safety of the repository is evaluated, to show that the repository is capable of protecting human health and the environment against ionising radiation in a long-term perspective.

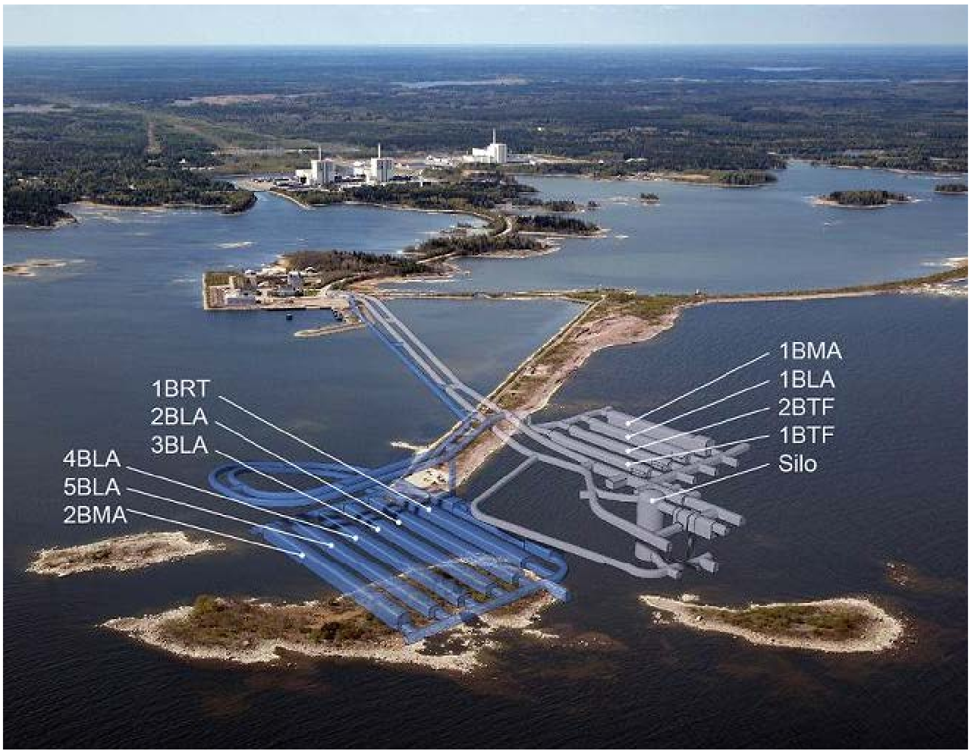

Figure 1-1. *The proposed extension of the SFR repository. The present SFR repository is located to the right (light grey colour) while the planned new tunnel system is shown to the left (light blue colour). The existing facility is situated about 60- 140 m below the seabed of the Baltic Sea, while the extention is proposed to reach c. 120 m below sea level.*

In this context, the hydrogeochemical evolution is a crucial factor in the safety assessment. The chemical composition of groundwater in the rock volume surrounding the repository is of importance to many variables that affect its performance (e.g. to evaluate the long-term concrete degradation processes, the long-time stability of the engineered barriers, etc) and the changes in the hydrochemical environment over time, during the expected evolution, must be addressed.

The hydrogeochemical evolution at repository depth will be strongly conditioned by the hydrogeology of the site which, in turn, depends upon the expected future climate evolution. In this report, a selection of reference groundwater compositions that may be expected to be in contact with the repository under different climate conditions, is presented. This selection is mainly based on the conceptual Hydrogeochemical model SFR v. 1.0 (Nilsson et al. 2011) performed as part of the SDM-PSU. This work establishes a detailed understanding of the hydrogeochemical conditions at the site and develops models for its description and visualisation. The focus was to describe the chemistry, origin and distribution of the groundwaters in the bedrock and the hydrogeochemical processes involved in their evolution, as well as the short term impacts since 1984 from the construction and operation of the present SFR repository.

Understanding the evolution of the groundwater system over time, i.e. since the last glaciation and more recently since excavation and construction of the SFR repository, showed that: 1) present day hydraulic conditions have preserved groundwater compositions and hydrochemical trends which replicate to a large extent what will occur during the next deglaciation (long term perspective), and 2) the future impact of extended excavations and underground construction on groundwater chemistry can be predicted from past to present day observations at the SFR site (short term perspective).

1.2 Objectives and scope

The main objective of this study was to estimate reference groundwater compositions around the SFR repository in Forsmark in periods of different climate domains, and submerged/emerged conditions. The impact of extended periods of a specific climate domain and shorelevel conditions is also assessed. The resulting reference groundwater compositions will be used in different modelling activities within the SR-PSU safety assessment.

As stated above, the basis for the selection of these reference groundwater compositions, in the selected climate domains, are the chemical analysis, compilations, reviews and conclusions available from the SDM-PSU but also from other research programmes, mainly the Site Characterisation Programmes in Forsmark and Laxemar (including groundwaters, GW, and near-surface groundwaters, NSGW). Additional chemical data from wells, experiments, different controlling sampling campaigns and the ulterior monitoring programmes (in Forsmark, Laxemar and SFR), and data from private wells in northern Uppland have also been considered, mainly for comparison.

1.3 Report layout

A summary of the present SFR hydrochemical conceptual model is presented in Chapter 2 and then Chapter 3 presents a short summary of the climate cases, describing the future climate evolution, as reported in SKB (2013b).

The main part of the work is presented in Chapter 4 with a detailed description of the procedure followed to decide the reference groundwater compositions that will be around the repository during periods of different climate domains and for submerged/emerged conditions.The final proposed compositions are compiled in tables in Chapter 5.

Finally, Appendix A, presents the sensitivity analyses performed to asses the effect of considering additional chemical data on the final results (data from wells, experiments, different controlling sampling campaigns, monitoring programmes and regional data from private wells in northern Uppland). Appendix B, describes the values proposed for the concentration of dissolved organic carbon (DOC) in groundwaters during the different climate domains. Appendix C includes a description of the structure and contents of the Excel file with the data table used for this work.

2 Conceptual model

2.1 General context

The present SFR hydrogeological and hydrogeochemical conceptual models integrate the past climate changes in the Forsmark region, and their effects on the recharge waters, with the major hydrogeological and hydrogeochemical features of the investigated SFR rock volume (Figure 2-1).

Past climatic changes, which in the Forsmark region have involved glaciations/deglaciations and marine transgressions/regressions, are the major driving forces for the long term hydrogeochemical changes in the bedrock through the successive penetration of old meteoric or old glacial waters (derived from temperate and cold climate events), and the more recent Weichselian dilute glacial melt-waters, the Littorina sea waters and the recent dilute meteoric waters. They are, therefore, of fundamental importance in understanding the palaeohydrogeological, palaeohydrogeochemical and present evolution of the groundwaters in the region. Based on the Quaternary evolution for the Forsmark region following the last deglaciation, an overall climatic-palaeohydrological evolutionary model has been proposed for the SFR area (Nilsson et al. 2011, SKB 2013a).

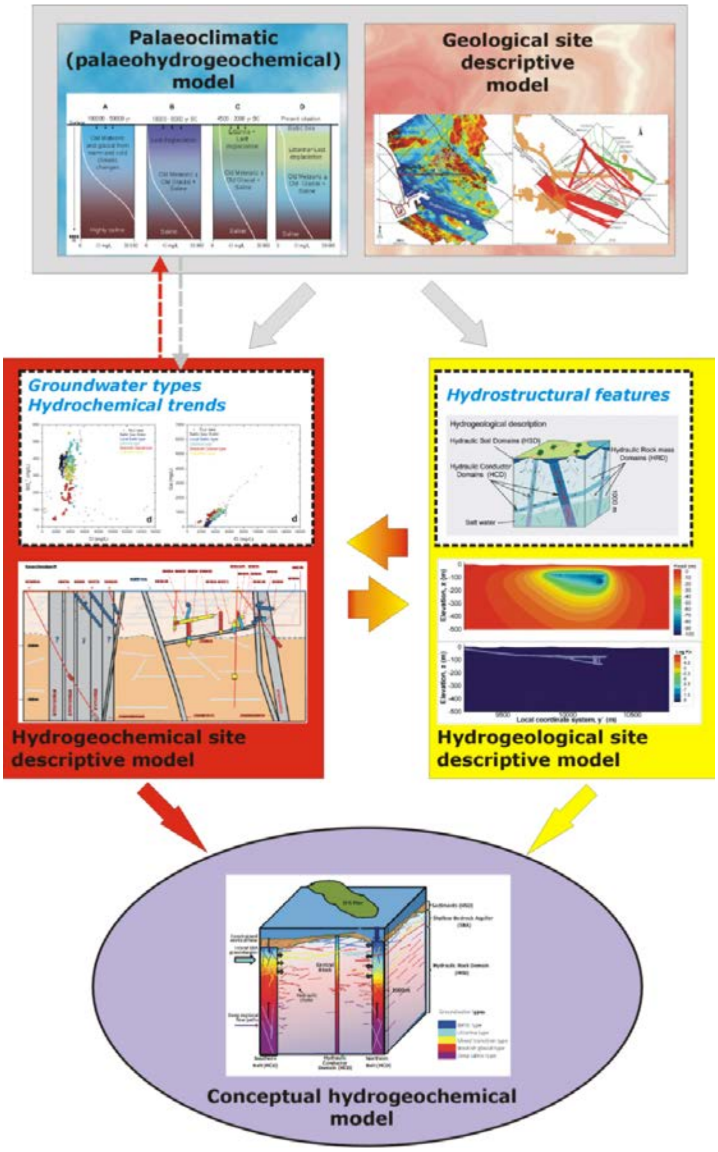

Figure 2-1. Sketch of the site descriptive models integrated in the present SFR conceptual hydrogeochemical model.

The hydrostructural properties of the bedrock control the flow paths and depths reached by the recharge waters and, thus, the degree of mixing with the previous, resident groundwaters. As a result, water types such as deep saline, glacial, marine and meteoric waters have intruded and mixed in a complex manner at various levels in the bedrock. In addition, the situation of the SFR (under the Baltic Sea) has led to the present intrusion of Baltic Sea waters due to the drawdown created by the SFR tunnel construction. This artificially imposed dynamic flow system is naturally more prevalent along major deformation fracture zones of higher transmissivity, whilst lower transmissive fractures together with the less transmissive bedrock masses between major deformation zones, still retain some evidence of the natural groundwater mixing patterns established prior to the SFR construction (Nilsson et al. 2011, SKB 2013a).

In this situation, to separate groundwaters of different origins and residence times in the SFR bedrock, a modified subdivision of the groundwaters (with respect to the one applied for the SDM-Site Forsmark) was proposed (Nilsson et al. 2011, SKB 2013a). The defined groundwater types were central to the explorative analyses and modelling approaches (such as mixing modeling or geochemical equilibrium modeling) performed to evaluate the chemical variations in the SFR groundwaters (studied during the Site Descriptive Modelling of the SFR, SDM-PSU). Furthermore, they facilitated interaction and integration with the geological and hydrogeological models making the construction of the aforementioned hydrogeochemical site descriptive model for the SFR site possible (Nilsson et al. 2011, Gimeno et al. 2011, SKB 2013a).

The hydrogeochemical conceptual model for the SFR has been presented with different degrees of detail and interdisciplinary integration, in the SDM-PSU report (SKB 2013a) and in the SFR hydrogeochemical site description version 1.0 (Nilsson et al. 2011). More specific works, focused on the mixing and reaction processes or in the mineralogical characters, are found in the background reports by Gimeno et al. (2011) and Sandström and Tullborg (2011), respectively. Next a summary of this model is presented as it has been the basis to construct and propose the reference waters compositions for the different climate domains.

2.2 Conceptual hydrogeochemical model

The present SFR hydrogeochemical conceptual model (Nilsson et al. 2011, SKB 2013a), integrating the major hydrogeological and hydrogeochemical features of the investigated SFR rock volume, has been based on the available hydrogeological 0–1,000 m depth conceptual model (Nilsson et al. 2011). The block model illustrated in Figure 2-2 includes colour coding of the main groundwater types in the three major flow path structures and in less transmissive discrete fractures which characterise the general SFR rock volume between these structures. The conceptual model is related to the palaeohydrological evolution summarised above and it is described as follows.

Based on the SDM-Site Forsmark groundwater data[1] (because no data below –400 m.a.s.l. elevation are available from the SFR area) the "initial" situation in this evolutionary sketch is represented by the presence of a saline non-marine groundwater type (highly saline), now ascribed to the deepest part of the bedrock (deep lilac color; Figure 2-2).This groundwater type is associated with the two highly transmissive deformation areas (i.e. the Southern and Northern boundary belts) and the central Hydraulic Conductor (a weak regional flow direction upwards is indicated by the upward pointing black arrows). A more subdued lilac colour, increasing in intensity with depth, represents the less transmissive rock volume between these structures characterised by few discrete fractures of low conductivity. Waters in these discrete fractures (and possibly also the rock matrix porewaters) probably represent salinities similar to the deepest groundwaters in the major conducting structures (i.e. deeper than about 700 m based on the SDM-Site Forsmark investigations). Saline non-marine

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[1] Data compiled and used during the site investigations carried out in Forsmark (SKB 2008b) for the application for the spent fuel repository (SR-Site; SKB 2011). We will refer to them as Forsmark site groundwaters, or, simply Forsmark groundwaters. The groundwater dataset used for the SFR Site Descriptive Modelling (SDM-PSU), although geographically included in the Forsmark area, do not correspond to the Forsmark SDM groundwaters and they will be referred as SFR site groundwaters, or, simply SFR groundwaters.

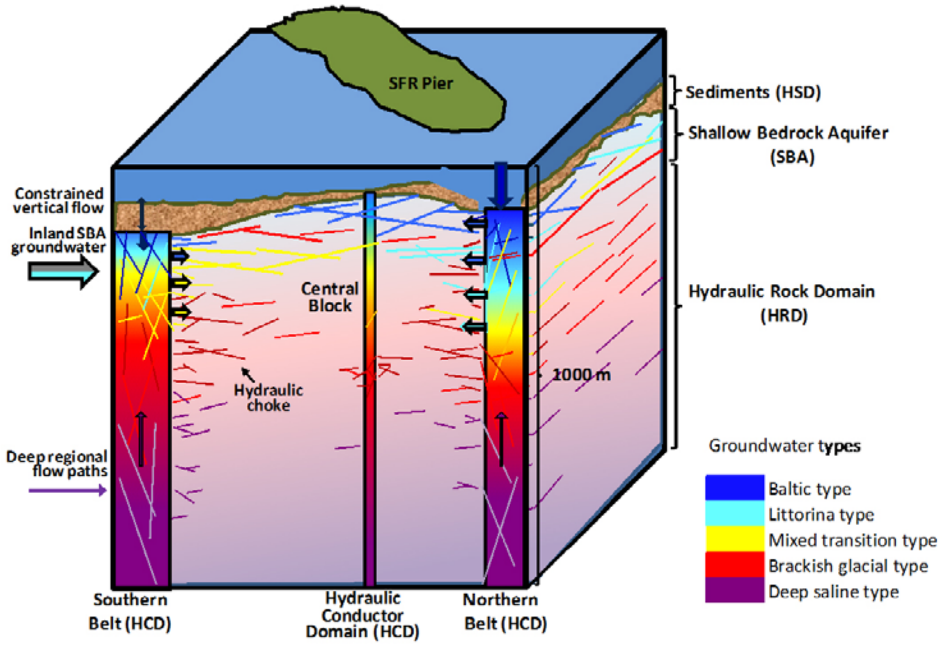

Figure 2-2. *Conceptual block model (0-1,000 m depth) integrating the major hydrogeological and hydrogeochemical features of the investigated SFR rock volume. The different groundwater types are indicated by the same colour scheme used in the other figures in this report with the exception of the deeper saline groundwater which is indicated by lilac and is not present as a dominant groundwater type in the SFR rock volume. See text for explanation to the different arrow types. AfterNilsson et al. (2011) and SKB (2013).*

groundwaters mixed with old meteoric groundwaters could be present at shallower depths and, presently, some preserved components of these old meteoric groundwaters may be present at intermediate depths (especially within the lower transmissive rock mass).

This situation was modified by the successive penetration of different recharge waters since the last glaciation:

- Introduction of glacial meltwaters particularly along the highly transmissive deformation zones but also into smaller, less conductive fractures or dead-end fractures heterogeneously distributed within the rock mass. The mixing with the older non-marine saline to brackish groundwaters (and components of old meteoric water) has given rise to the brackish-glacial groundwater types (bright red color; Figure 2-2).
- This was followed by the infiltration of the Littorina Sea water and its mixing with different portions of glacial meltwater giving rise to the Littorina type groundwater (turquoise colour). The Littorina Sea water entered preferentially along the more highly conducting fracture zones, i.e. the same zones that facilitated the glacial meltwaters. Mixing of these Littorina type waters has occurred to different degrees with the earlier brackish-glacial groundwaters producing the mixed brackish water (transition) type groundwaters (yellow colour; Figure 2-2). There are locations where mixing has not occurred and where the brackish-glacial groundwaters have remained at shallower levels in the bedrock (‘pockets’) shielded from the passage of the later Littorina type groundwaters; this is schematically indicated as red infilled fractures at higher levels than the maximum depths achieved by the Littorina type groundwaters. Littorina-type groundwaters may also have been preserved under special conditions and this is also indicated by the turquoise colour of some of the near-surface discrete fractures.
- Modern Baltic Sea water (dark blue colour; Figure 2-2) is most probably a recent component that has intruded via the highly transmissive deformation zones comprising the Northern and Southern boundary belts due to the drawdown effect of the SFR facility construction. However, sea-bottom sedimentation has been much more developed (i.e. thicker) above the Southern boundary belt compared with the Northern one, allowing a greater volume of Baltic Sea type water to preferentially infiltrate to the latter (indicated by the larger and thicker downward pointing blue arrow; Figure 2-2).

As indicated by the concentration of short thick horizontal arrows from the upper approximately 400 m parts of the Northern and Southern boundary belts, the SFR drawdown has gradually pulled in groundwaters along conducting fracture zones into the Central block area and towards the SFR site. These groundwaters, already the product of natural mixing processes affecting brackish-glacial and Littorina type waters, therefore have undergone additional anthropogenic mixing involving a Baltic Sea input and this has been compounded by the increased flow resulting from drawdown effects.

The input from the Northern belt to the Central block area of mixed groundwaters with components of Brackish-glacial, Littorina and Local Baltic type waters is indicated by the dark blue of the Baltic Sea close to the surface in the Northern belt, and a dominant turquoise Littorina component at greater depth. The presence of a brackish-glacial component (red) is also assumed to occur at still greater depths mixed with Littorina-type groundwaters to give rise to transition type groundwaters (yellow). The Southern belt is considered to be less transmissive because of the thick sediment cover, and the mixing processes are, therefore, slower, more thorough and widespread (compare the extent of the yellow colouring between the two belts).

The conceptual model also shows a lateral flow direction to the Southern boundary belt from the near-surface sheet joints (Shallow Bedrock Aquifer, SBA; Figure 2-2) which may have transported mixtures of modern meteoric water with some residual Littorina type water from inland, i.e. from the north-eastern part of the Forsmark area. However, this is based on too few data and may simply reflect the hydrogeological and hydrogeochemical heterogeneity of the bedrock system.

3 Future climate evolution

The handling of climate and climate-related processes in safety assessments must be tailor-made for each repository concept and waste type to be analysed (Näslund et al. 2013). Further, climate is not predictable on a 100 ka timescale. Therefore, *a range* of future climate developments must be considered in the safety assessment in order to cover the uncertainty in future climate development. This range is determined based on scientific knowledge on past, present and future climate evolution, as well as knowledge of which processes are of importance for evaluating the functioning of the repository concept under consideration (SKB 2013b).

The future Forsmark climate developments (climate cases) defined for SR-PSU are described as a succession of climate-driven process domains ("climate domains"), where such a domain is defined as "a climatically determined environment in which a set of characteristic processes of importance for repository safety appear". For Forsmark, a site on the Baltic Sea coast, a set of three climate domains were identified. These are denominated: 1) the temperate climate domain; 2) the periglacial climate domain; and 3) the glacial climate domain. For a detailed description of these domains, see SKB (2013b).

A total of four climate cases are defined in SR-PSU. The first three cases represent different levels of cumulative carbon emissions due to human activities. From low to high level CO_2 emissions, the climate cases are: the *"early periglacial climate case"*, the *"global warming climate case"* and the *"extended global warming"* (SKB 2013b). To supplement this range of future climate developments a climate case based on a reconstruction of the last glacial cycle was defined. The *Weichselian glacial cycle climate case* represents a climate development dominated by natural variability as manifested during the past c. 100 ka (SKB 2013b).

The main difference among the different climate cases is the length or duration of the successive warm and cold periods (climate domains; Figure 3-1). For the "*global warming climate case*", the current interglacial is extended to 50 ka AP (after present) due to human intervention and natural climate variability is assumed after this. In the early periglacial climate case the current interglacial is interrupted at 15.5 ka BP by a shorter period of periglacial climate conditions; temperate conditions are assumed to prevail afterwards until 50 ka AP and natural climate variability is assumed after that.

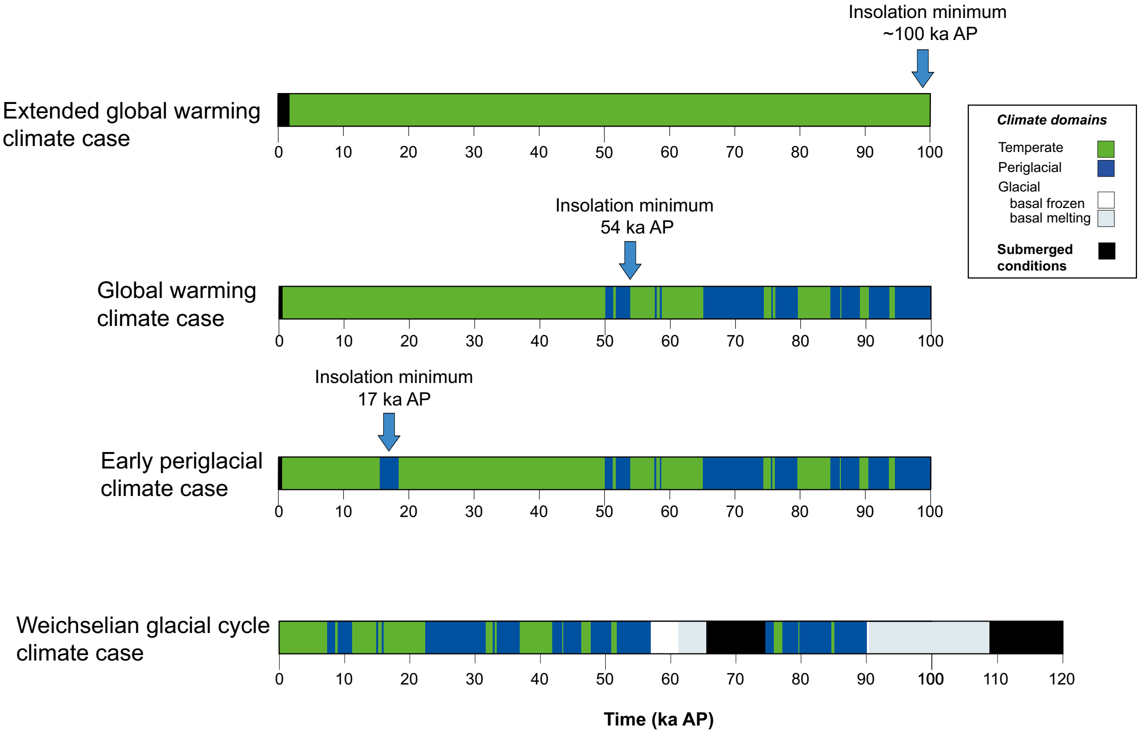

***Figure 3-1.** Summary of the four future climate cases considered in the SR-PSU safety assessment (taken from SKB 2013b). The cases go from warmer/wetter at the top to colder/dryer climates at the bottom.*

Finally, temperate conditions are assumed for the complete 100 ka in the case of the "*extended global warming climate case*". The *"Wechselian glacial cycle climate case"* represents the repetition of the climate evolution reconstructed for the last glacial cycle.

Table 3-1 presents a summary of the total duration of the different periods (climate domains) for the four climate cases considered in SR-PSU and shown in Figure 3-1. The definition of these climate domains can be summarised as follow: In the *temperate climate domain* no regions exist where permafrost or ice sheets are present. This domain has the warmest climate among the three considered. During this climatic period, the site may at times be submerged under the Baltic Sea. Strictly speaking, the *periglacial climate domain* is characterised by regions with permafrost but without the presence of an ice sheet. The climate is colder than the temperate climate domain and warmer than the glacial climate domain. Within the periglacial climate domain, the site may also, at times, be submerged by the sea. The *glacial climate domain* is characterised by regions that are covered by glaciers or ice sheets which may, in some cases, be underlain by sub-glacial permafrost. The glacial climate domain has the coldest climate among the three considered climate domains. For further descriptions of the climate domains that are used to describe the climate cases, see SKB (2010a, Section 1.3.2).

The three different climate domains, together with the shorelevel which determines if the repository location is submerged or emerged from the Baltic Sea, occur succesively in the different climate cases. The prevailing climate domain conditions the groundwater composition around the repository. In the following, reference groundwater compositions around the repository in each of these different climate domains and for submerged/emerged conditions are estimated. When possible, the hydrochemical effects conditioned by the length of the periods of different climate domains have been discussed.

Table 3-1. Summary of duration of climate domains for the four climate cases considered in the SR-PSU safety assessment (taken from SKB 2013b).

Climate case	Temperate climate domain (ka) (percent of 100 ka assessment time)	Periglacial climate domain (ka) (percent of 100 ka assessment time)	Glacial climate domain (ka) (percent of 100 ka assessment time)	Submerged conditions (ka) (percent of 100 ka assessment time)
Extended global warming	100 ka (100%)	0 ka (0%)	0 ka (0%)	1.8 ka (2%)
Global warming	69 ka (69%)	31 ka (31%)	0 ka (0%)	0.6 ka (<1%)
Early periglacial	66 ka (66%)	34 ka (34%)	0 ka (0%)	0.6 ka (<1%)
Weichselian glacial cycle	31 ka (26%)	41 ka (34%)	28 ka (24%)	19 ka (16%)

4 Groundwater composition for the different climate domains

As indicated in the previous section (Figure 3-1) four climate cases, describing different future climate developments, are analysed in the the SR-PSU safety assessment (SKB 2013b) and the main difference among them is the length or duration of the successive warm and cold periods (climate domains), these being: temperate, periglacial and glacial. In this section three reference groundwater compositions are proposed to represent the hydrogeochemical conditions around the repository under each of these domains.

Two possible situations are considered for the temperate domain, the case of the site being under the Baltic Sea (submerged as today) and the case of the site not covered by sea water due to the shoreline displacement. In the first case, an inflow of brackish-saline groundwater (similar to the situation at present) will dominate and this will be the first reference composition. In the second case, land uplift will have proceeded so far that the groundwater flowing into the repository will be fresh (non-saline). This will be the second reference water and it will have a composition similar to that found today in wells in the area (Östhammar Municipality). For the periglacial climate domain, under permafrost conditions, no great changes are expected in the salinity of the groundwater, that is, a non-saline groundwater (similar to the second reference water expected during the temperate domain) is expected. Some discussion about its composition will also be presented in this section. Finally, for the glacial domain the repository will be located beneath a warm-based ice sheet, the inflowing meltwater will result in low salinity in the repository. This will be presented as the third reference water.

The basis for the selection of the reference groundwater composition for these climate domains are the chemical analyses, compilations, reviews and conclusions available from different research programmes, mainly the Site Charaterisation Programmes in Forsmark, Laxemar and SFR (SDM-Site Forsmark, SDM-Site Laxemar and SDM-PSU), including groundwaters (GW) and near-surface groundwaters (NSGW, from 0 to 20 m depth). Additional chemical data from wells, experiments, different controlling sampling campaigns and the ulterior monitoring programmes (in Forsmark, Laxemar and SFR), and regional data from private wells in northern Uppland (defined by N: 6633169 - 6725589, E: 627152 -733165, Sweref99TM) have also been considered. Depending on the water that is looked for as a reference, the dataset used is different and it is indicated and justified in the next sections. However, in general, the criteria has been to use those data already categorised in the previous hydrogeochemical works, considered as representative samples of the system. In any case, a comparison of the results obtained when using different and supplementary datasets has been performed and it is included in the Appendix A. The specific set of data used in each case (and the uncertainty analyses performed using different sets of data) is indicated.

In all the cases, for every climate period considered, the values for a specific set of geochemical parameters are proposed for a hypothetical groundwater around the repository under that specific climate domain. These parameters include: chloride, sulphate, sodium, calcium, magnesium, potassium, silica, the main parameters of the carbonate system (alkalinity and pH) and Eh. They are, in one way or another, included in the performance assessment calculations and thus, it is necessary to assess their possible contents in the groundwaters related with the different climate domains.

The concentration of dissolved organic carbon (DOC) is of special interest for microbiological interpretations. It may favour reducing conditions through microbial activities but it may also have detrimental effects (e.g. the formation of organic complexing compounds and organic colloids might enhance the potential for radionuclide transport; Salas et al. 2010, Gimeno et al. 2010). Unfortunately, the amount of data and their reliability is not as high as for the rest of the chemical constituents and moreover, there is very little information concerning the DOC contents and the chemical characteristics of groundwaters related to permafrost and glacial conditions. Therefore, a special treatment has been given to this parameter and it is included in Appendix B.

4.1 Groundwater composition for the temperate climate domain

4.1.1 Temperate climate domain with the repository submerged under the sea

During this climate domain, the situation of the repository will be similar to the situation at present, with the SFR covered by the Baltic Sea, and the groundwater around the repository characterised as a brackish saline groundwater with chloride contents between 2,800 and 5,500 mg/L (Nilsson et al. 2011, Gimeno et al. 2011).

In the previous SFR safety assessment (SFR 1; SKB 2008a), the reference composition selected for the penetrating brackish-saline groundwater after saturation of the repository was based on (a) measurements made during the construction of SFR 1 (1984–1986), (b) data from the monitoring programme for SFR 1 (1989–1999) and (c) geochemical calculations (Höglund 2001). Geochemical calculations were used to adjust the water composition to be in thermodynamic equilibrium with some selected minerals. The contents of calcium and magnesium were adjusted to be in equilibrium with calcite and dolomite. Moreover, a silica content (equilibrated with quartz) was added to make the results on the degradation of concrete calculation more accurate.

For the present assessment (SR-PSU) different sources of data are used. Considering that the repository will be submerged under the sea during this climate domain, the assumption made here is that the brackish-saline water in contact with the repository will be similar to the brackish-saline waters there at present. Therefore, the most suitable set of data to be considered here is the set of groundwater samples from the SFR (Gimeno et al. 2011, Nilsson et al. 2011). However, due to its proximity, the available data from the SDM-Site Forsmark groundwaters (Laaksoharju et al. 2008, Gimeno et al. 2008) have also been considered as a comparative term.

The compiled dataset used for the SFR-extension modelling work (SDM-PSU) included (Nilsson et al. 2011):

- Groundwater data from the hydrogeochemical investigation programme in the SFR extension project comprising a total of 15 borehole sections in five cored drilled and three percussion boreholes.
- Groundwater data extracted from the SKB database Sicada related to the period 1984 to October 2010; altogether a total of 45 borehole sections in 18 early boreholes drilled from the SFR tunnel system.
- Late supplementary data obtained in the autumn of 2010 from complementary investigations within the SFR extension project (Nilsson 2011), as well as from the regular annual control programme in the SFR.
- Data representing three boreholes from the SDM-Site Forsmark located within the SFR extension regional model volume.

The groundwaters in the SFR dataset cover a depth down to –250 m.a.s.l., and some single sampling locations at –300 and –400 m.a.s.l., and represent a relatively limited salinity range (1,500 to 5,500 mg/L chloride). However, the δ^{18}O values show a wide variation (–15.5 to –7.5‰ V-SMOW) similar to that reported for the SDM-Site Forsmark groundwaters (Laaksoharju et al. 2008). At the SFR, marine indicators such as Mg/Cl, K/Cl and Br/Cl also show relatively large variations considering the limited salinity range. This information together with palaeoclimatic considerations were used by Nilsson et al. (2011) to differentiate the groundwaters into four major types: 1) local Baltic Seawater type, 2) Littorina type water with a glacial component, 3) brackish-glacial water type, and 4) mixed brackish water (transition type). These water types are used in the following plots shown below with the distribution of the different parameters in the SFR system.

For the final selection of the reference composition, two sets of data from SFR have been considered: (a) the total of the analysed samples, down to –400 m.a.s.l. (including the small set of more dilute waters found at about –300 m depth at the SFR); and (b) only considering the groundwaters located above –200 m depth (ignoring the set of dilute groundwaters).

The so-called Forsmark dataset used here includes the samples taken and studied during the SDM investigations at the Forsmark site, and the monitoring samples taken after that. As for the SFR groundwater samples, two different sets of data have been used from the Forsmark dataset:

(c) samples from all depths, (d) only samples down to –200 m depth (more similar to the SFR location). Moreover, in both cases (c and d), two different groups have been analysed: 1) only the samples categorised as 1, 2, 3 and 4 (quality suitable for modelling, as defined for the SDM investigations; c.f. Smellie et al. 2008); and 2) all the samples (this case is commented in Appendix A).

Dissolved chloride concentrations

The main hydrogeochemical data included in the SFR-extension modelling work (SDM-PSU) represent the depth range –20 to –400 m.a.s.l. (though most of the data correspond to shallow depths above –250 m.a.s.l.; Figure 4-1a) where the chloride concentration varies between 1,600 and 5,380 mg/L. However, only a few data points are below 2,800 mg/L Cl (the concentration of the present Baltic Sea) or exceeding 4,500 mg/L Cl (corresponding to the typical Littorina type composition identified from the SDM-Site Forsmark investigation). All of the latter were observed prior to 1995 since impacts from the SFR facility have caused dilution with time (Nilsson et al. 2011).

The most dilute brackish groundwater of the local Baltic type is found at shallow depths down to 100 m while the groundwater with the lowest salinity (1,600 mg/L Cl) is of the Brackish-glacial type and found at approximately 240 m depth (see Figure 4-1a with the groundwater type coding). The most saline groundwater is generally found at intermediate depths (100–200 m) and represents the brackish marine Littorina type.

Overall, groundwaters found down to 200 m depth define a range between 2,590 and 5,380 mg/L Cl, which could be considered representative of the groundwaters around the repository when submerged under the sea during a temperate climate domain (Figure 4-10a, b, Table 4-1 and Table 4-2).

Dissolved sulphate concentrations

Dissolved sulphate contents in the SFR groundwaters show a wide variation, ranging from 49.4 to 557.2 mg/L (Table 4-1 and Figure 4-10a, b) and their trends with respect to depth (Figure 4-1b) and chloride contents are closely similar to those of the Forsmark groundwaters (Gimeno et al. 2011, Nilsson et al. 2011).

The highest sulphate concentrations are associated with groundwaters with clear Littorina signatures and with chloride contents about 5,000–5,500 mg/L (Gimeno et al. 2011), as described for the Forsmark groundwaters. In the upper 200 m depth, sulphate contents in the SFR groundwaters range from 74 to 557.2 mg/L, very similar values to those observed in the Forsmark groundwaters at similar depths (Table 4-1, Figure 4-1b and Figure 4-10b and d). Thus, this range could be selected for the sulphate concentrations (Table 4-1 and Table 4-2).

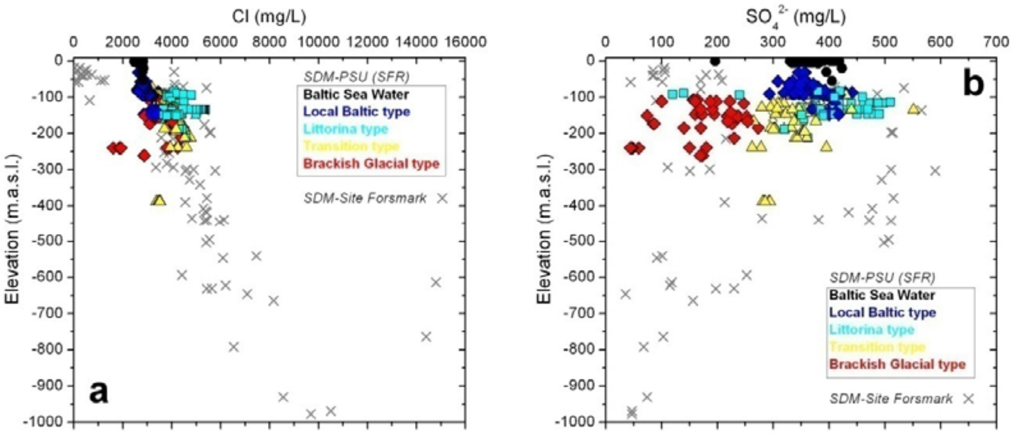

Figure 4-1. Distribution of chloride (a) and sulphate(b) with depth in the SFR (SDM-PSU) groundwaters (Nilsson et al. 2011). The samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011). Groundwaters from the Forsmark site (SDM-Site Forsmark) down to 1,000 m are also included in the plots (grey x).

Table 4-1. Statistical values for the waters taken at all depths in the SFR system (Set a), only down to 200 m at the SFR (Set b), in the Forsmark site at all depths (Set c) and only down to 200 m at Forsmark site (Set d). These groups of waters have been used to select the Reference Water for the temperate climate domain when the repository is under the sea. Only groundwaters from categories 1 to 4 have been included in the Forsmark site datasets.

	Total No.	Mean	Standard Deviation	Min	Median	Max	P0.1	P5	P95	P99.9
Set a (SFR groundwaters at all depths)										
pH	97	7.58	0.14	7.3	7.55	8	7.3	7.4	7.86	8
Eh	54	–26.72	108.30	–190	40	110	–190	–190	110	110
Na	349	1,461.09	217.90	658	1,470	1,920	658	1,100	1,780	1,920
K	342	13.51	8.83	3.8	10.9	60	3.8	5.2	32.2	60
Ca	351	676.23	276.51	87.4	704	1,220	87.4	207.3	1,100	1,220
Mg	349	146.62	46.10	30.4	139	290	30.4	90	258	290
HCO_3^-	330	103.18	21.97	40	107	157	40	64.7	134	157
Cl	351	3,675.45	702.84	1,600	3,700	5,380	1,600	2,750	5,000	5,380
SO_4^{2-}	346	368.12	97.19	49.4	394.0	557.2	49.4	160.0	473.3	557.2
SiO_2	342	11.11	1.86	2.6	10.9	17.2	2.6	8.6	14.0	17.2
Set b (SFR groundwaters down to 200 m depth)										
pH	87	7.56	0.11	7.3	7.54	7.86	7.3	7.4	7.73	7.86
Eh	54	–26.72	108.30	–190	40	110	–190	–190	110	110
Na	328	1,482.33	191.62	850	1,480	1,920	850	1,161	1,786	1,920
K	322	13.78	8.99	3.8	11	60	3.8	5.2	32.2	60
Ca	330	677.58	275.11	87.4	707.5	1,220	87.4	206	1,100	1,220
Mg	328	150.53	43.62	79	140	290	79	96	260	290
HCO_3^-	309	104.82	21.55	40	109	157	40	66	134	157
Cl	330	3,717.71	660.60	2,590	3,730.5	5,380	2,590	2,791	5,000	5,380
SO_4^{2-}	325	378.79	84.99	74.0	395.5	557.2	74.0	194.1	476.3	557.2
SiO_2	321	11.08	1.88	2.6	10.9	17.2	2.6	8.6	13.9	17.2
Set c (Forsmark SDM groundwaters at all depths; only categories 1 to 4)										
pH	71	7.49	0.38	6.78	7.42	8.4	6.78	6.93	8.21	8.4
Eh	14	–211.00	43.63	–281	–201.5	–143	–281	–281	–143	–143
Na	139	1,452.75	656.55	64.6	1,570	3,130	64.6	229	2,290	3,130
K	139	23.53	15.05	4.88	20.8	67.8	4.88	6.02	58.7	67.8
Ca	139	1,111.44	1,255.03	23.9	860	6,520	23.9	33.7	3,980	6,520
Mg	139	105.33	80.54	3.87	106	287	3.87	7.57	242	287
HCO_3^-	139	165.04	136.70	5.72	126	473	5.72	8.42	450	473
Cl	139	4,278.76	3,041.14	15.7	4,120	15,000	15.7	145	10,500	15,000
SO_4^{2-}	139	292.05	171.44	25.32	320.56	587.19	25.32	47.63	560.23	587.19
SiO_2	139	13.96	3.87	2.61	13.99	33.80	2.61	8.64	20.92	33.80
Set d (Forsmark SDM groundwaters down to 200 m depth; only categories 1 to 4)										
pH	29	7.37	0.26	6.87	7.4	7.81	6.87	6.95	7.75	7.81
Eh	2	–191.50	4.95	–195	–191.5	–188	–195	–195	–188	–188
Na	69	1,094.81	659.70	64.6	1,240	2,210	64.6	156	2,000	2,210
K	69	28.36	17.65	4.88	26	67.8	4.88	5.64	60	67.8
Ca	69	423.37	410.83	23.9	311	1,570	23.9	30.2	1,220	1,570
Mg	69	111.19	82.61	6.91	132	287	6.91	7.57	246	287
HCO_3^-	69	257.25	132.53	61.5	236	473	61.5	98.8	461	473
Cl	69	2,474.31	1,891.49	15.7	2,630	5,980	15.7	60.8	5,421.7	5,980
SO_4^{2-}	69	297.51	164.80	25.3	338.5	587.2	25.3	47.6	548.2	587.2
SiO_2	69	14.25	3.46	2.6	14.4	21.4	2.6	10.1	19.1	21.4

Table 4-2. Composition of penetrating brackish-saline groundwater and variation ranges for the paremeters of interest (mainly based on measurement data presented by Nilsson et al. (2011) and Gimeno et al. (2011)) for the temperate climate domain when the repository is submerged under the sea[2]. Ion concentrations in mg/L. Data from previous assessments are shown for comparison, proposed values are in bold and the maximum and minimum values are between brackets.

	This Assessment			**Wikberg 1999[1]**	**Safety analysis SFR 1[1]**
	Proposed composition	**Range**			
		all SFR samples	**SFR samples down to –200 m**		
pH	7.3	6.6–8.0	6.6–8.0	**7.5** (6.5, 7.8)	**7.3** (6.5–7.8)
Eh	–225	–100 to –350	–100 to –350	**–** (+50, –300)	**Red.** (–100, –400)
Cl	3,500	1,600–5,380	2,590–5,380	**5,000** (3,000, 6,000)	**5,000** (3,000, 6,000)
SO_4^{2-}	350	49.4–557.2	74–557.2	**500** (20, 600)	**500** (20, 600)
HCO_3^-	90	40–156	40–157	**100** (40, 110)	**100** (40, 110)
Na	1,500	658–1,920	850–1,920	**2,500** (1,000, 2,600)	**2,500** (1,000, 2,600)
K	20	3.8–60	3.8–60	**–**	**20** (6, 30)
Ca	600	87–1,220	87–1,220	**1,000** (800, 1,600)	**430** (200, 1,600)
Mg	150	30.4–290	79–290	**300** (100, 300)	**270** (100, 300)
SiO_2	11	2.6–17.2	2.6–17.2	**–**	**5.66**

[1] Data from Höglund (2001). Chemistry data for the assessment in Safety analysis SFR 1 are also presented in Table 6-5 from SKB (2008a).

Carbonate system: pH, calcium and alkalinity

As already indicated before, the available groundwater data for SFR were recorded at different occasions over the last 25 years and in the case of pH it means that the type of measurement, and therefore its quality, varies considerably. Out of the 416 groundwater samples studied in the SFR extension project (SDM-PSU), 245 have laboratory measurements and 40 do not have any pH value. Field pH measurements have been performed only for 78 samples. Data representing 12 pH (and Eh) values from Chemmac measurements, corresponding to seven borehole sections, are also available. The same selected Chemmac pH has been used for all the samples corresponding to the same section and date (53 samples in total; Gimeno et al. 2011).

Thus, field measurements for pH are available only for 19% of the total number of samples. As this situation represents a source of uncertainty in speciation solubility-calculations (Gimeno et al. 2011), theoretical pH values were calculated for the SFR groundwaters by adding or extracting the amount of CO_2 gas necessary to reach calcite equilibrium, which was assumed to represent the original groundwater conditions.

All measured pH in the SFR groundwaters ranges from 6.6 to 8.0 (Figure 4-2; values up to 8.3 have been measured in the Baltic Sea waters). In general, values determined in the field show a narrower range (7.3 to 8.0; Table 4-1 and Figure 4-10e) than the pH values measured in the laboratory. The calculated pH values (assuming calcite equilibrium) are also within a narrower range, between 7.0 and 7.7.

No clear correlation with depth, neither for measured nor for calculated pH values, is apparent and, thus, this conclusion is not affected by the pH uncertainties (Gimeno et al. 2011). This situation may be the result of the heterogeneity of the system and the frequent horizontal dispersion of this parameter in the examined sections, possibly due to the evolution of the groundwaters over time.

Field pH measurements in the groundwaters from the SDM-Site Forsmark range from 6.8 to 8.4 but most of the available values correspond to depths greater than 200 m (Figure 4-2a). The scarce pH data at shallower levels are between 6.9 and 7.8 (Table 4-1). Overall, from these data a pH value of 7.3 could be selected with a range from 6.6 to 8.0 (Figure 4-10e, Table 4-1 and Table 4-2).

Calcium contents in the SFR groundwaters range from 87.4 to 1,220 mg/L (Table 4-1, Figure 4-3 and Figure 4-10a, b). The lowest calcium concentrations are associated with some Local Baltic type groundwaters (87–90 mg/L at 82.9 m depth). However, although some of these Local Baltic Type waters show the lowest calcium contents, in most of them the contents are clearly higher

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[2] This composition is also assumed for the periglacial climate domain when the repository is covered by the sea (Section 4.2).

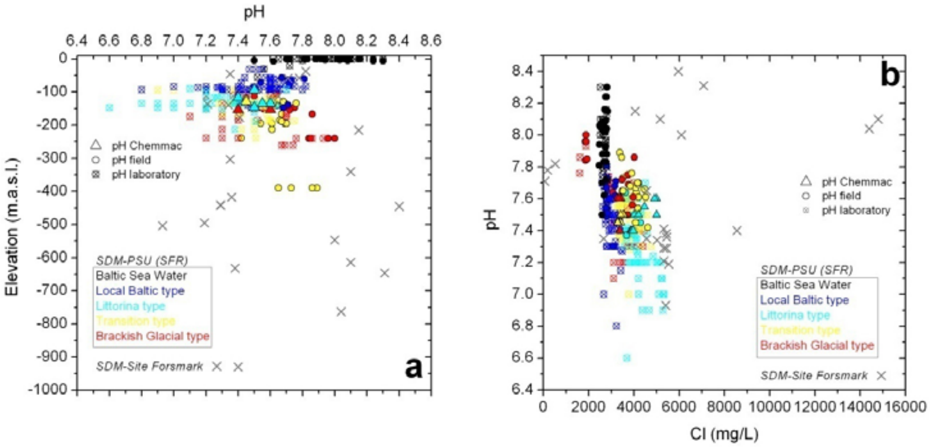

Figure 4-2. *Measured pH values with respect to depth (a) and chloride (b) in the SRF groundwaters. The plots show these data integrated in the general distribution of the Forsmark SDM groundwater data. The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).*

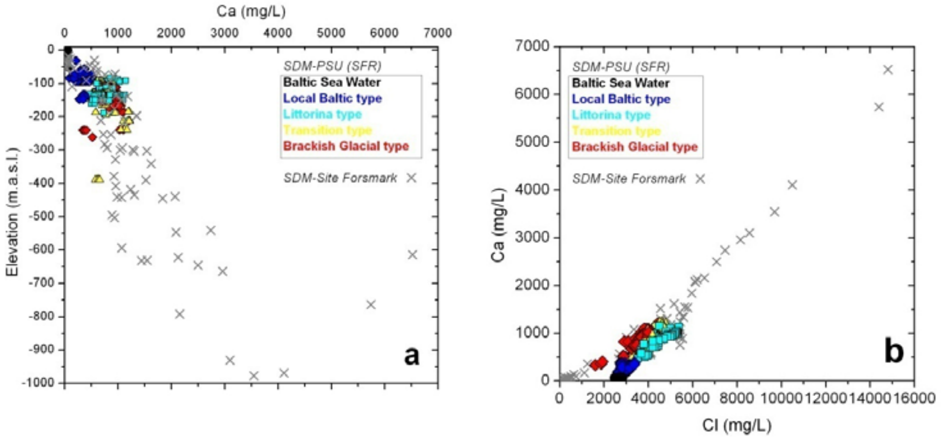

Figure 4-3. *Calcium contents vs depth (a) and chloride contents (b) in the SFR groundwaters.The plots show these data integrated in the general distribution of the Forsmark SDM groundwater data.The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).*

(between 200 and 600 mg/L) than the present Baltic Sea waters (around 75–80 mg/L; black dots in Figure 4-3a) and with a rough positive correlation with chloride contents (Figure 4-3b). Therefore, though these local Baltic type waters have been affected by heterogeneous reactions (e.g. calcite dissolution-precipitation, cation exchange), a mixing control seems to be still noticeable on them.

Littorina type groundwaters usually show higher contents than the Local Baltic type, reaching values around 1,200 mg/L. The highest calcium concentrations are found in some Mixed Transition type groundwaters in the upper 200 m, with values around 1,220 mg/L (Figure 4-3a and Figure 4-10a, b). The same range of values and depths were indicated for the Forsmark site groundwaters (Figure 4-10d).

From all these data, a range of 87.4–1,220 mg/L for calcium concentrations can be proposed for this brackish-saline reference water (Table 4-1 and Table 4-2).

The bicarbonate concentrations in the SFR groundwaters range from 40 to 157 mg/L (Table 4-1, Figure 4-4 and Figure 4-10a, b) and their trends with respect to depth and chloride contents almost perfectly reflect those of the Forsmark site groundwaters (Figure 4-4). However, in SFR, bicarbonate does not show the high concentrations found in the fresh and mixed groundwaters from the upper part of the system (above 150 m depth; Figure 4-4a) in the Forsmark area where the carbonate

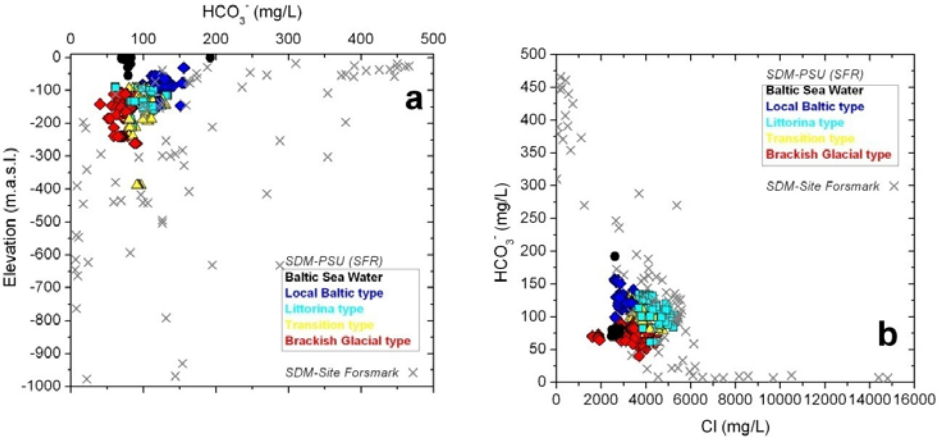

Figure 4-4. *Bicarbonate contents vs depth (a) and chloride contents (b) in the SFR groundwaters.The plots show these data integrated in the general distribution of the Forsmark SDM groundwater data.The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).*

system and the biogenic production of CO_2 related to the infiltration of meteoric waters, are very active (Gimeno et al. 2008, 2009).

The highest bicarbonate contents in the SFR area are found in the shallow brackish marine groundwaters of Local Baltic type (Figure 4-4a) and they are usually higher than the range between 70–90 mg/L usually found in the Baltic Sea water at the surface. Littorina type groundwaters show variable and also high bicarbonate contents (reaching 134 mg/L; Figure 4-4a), frequently higher than the estimated value for Littorina marine waters (92.5 mg/L).

Some of the Mixed Transition type groundwaters also show high bicarbonate contents and the Brackish Glacial groundwaters have concentrations well above 50 mg/L. The extremely low values found in the Forsmark site dataset (Figure 4-4a and Figure 4-10d) for the same range of depth do not appear in the SFR groundwaters.

The highest and more variable contents in bicarbonate are found in the upper 200 m (Figure 4-4a) and, thus, a range between 40 and 157 mg/L (Table 4-1 and Table 4-2) could be proposed for the bicarbonate concentrations.

Dissolved sodium concentrations

Sodium concentrations in the SFR groundwaters range from 658 to 1,920 mg/L (Figure 4-5). The lowest values are associated to the “isolated” Glacial type groundwaters located at 240 m depth (see Gimeno et al. 2011 for further details). The highest values (from 850 to 1,920 mg/L) have been measured in the upper 200 m depth, associated with the Littorina type groundwaters (Figure 4-5).

At similar depths in the Forsmark site groundwaters, sodium shows a wider range, from 64.6 to 2,210 mg/L (Figure 4-5). The lowest values are associated with fresh, dilute groundwaters (Laaksoharju et al. 2008), not present in the SFR area, whereas the highest values are associated with groundwaters with a more intense Littorina imprint than those in the SFR zone. Thus, from the upper 200 m in the SFR site, a range between 850 and 1,920 mg/L (Table 4-1 and Table 4-2) for sodium could be proposed.

Dissolved magnesium concentrations

The magnesium concentration emphasises the marine influence in most groundwaters within the SFR model volume (Nilsson et al. 2011). The magnesium content varies between 30.4 to 290 mg/L and the lowest concentrations (< 7 mg/L), observed in the fresh groundwaters from the Forsmark site (during the site investigation; Figure 4-6a, b), are absent in the samples from the SFR site as there are not fresh-type groundwaters in this area.

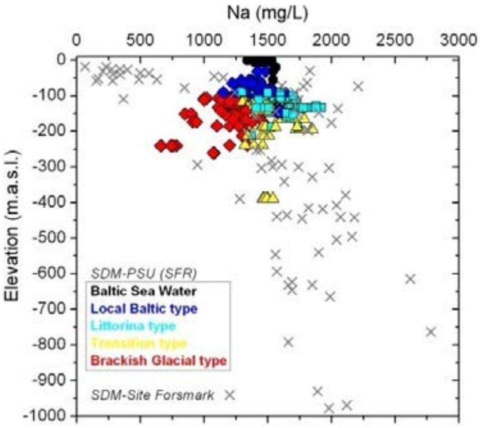

Figure 4-5. Distribution of sodium with depth in the SFR groundwaters. Forsmark SDM groundwaters down to 1,000 m are also included in the plots. The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).

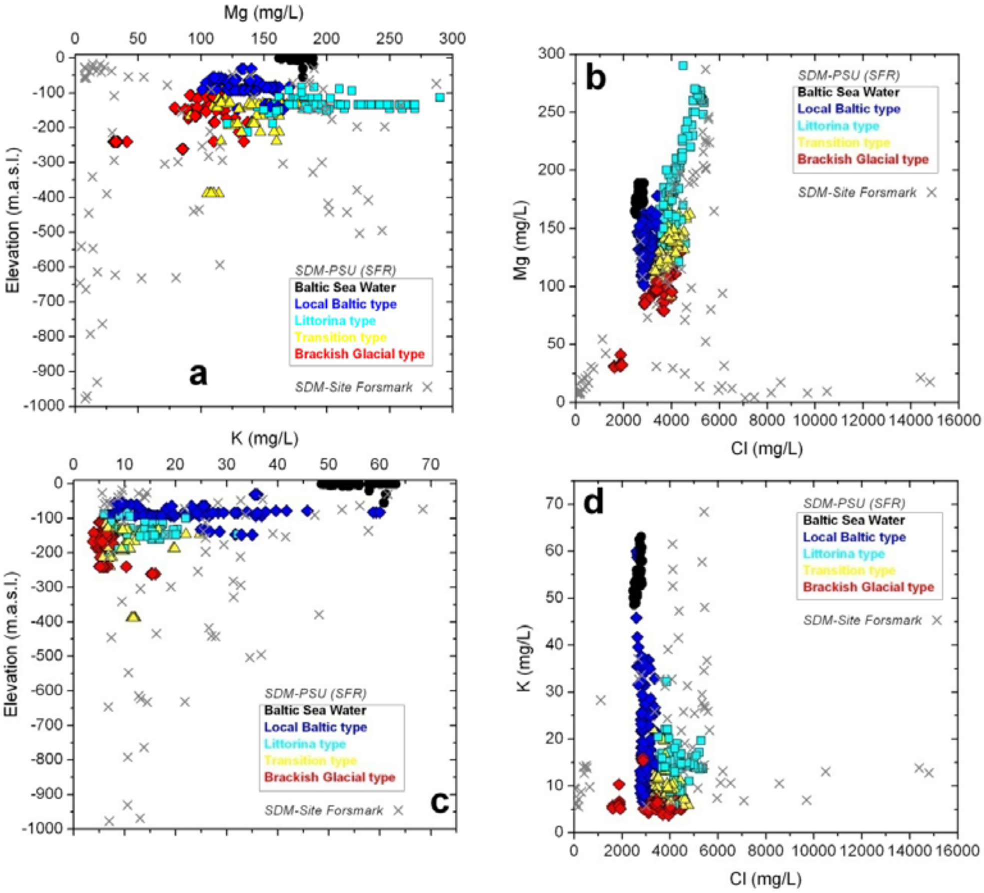

Figure 4-6. Distribution of magnesium (a) and potassium (c) with depth and with respect to chloride (b and d) for the SFR groundwaters(Nilsson et al. 2011). Forsmark SDM groundwaters down to 1,000 m are also included in the plots. The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).

The younger marine groundwaters of the local Baltic type generally show magnesium concentrations between 80 and 150 mg/L and are found down to depths of about 100 m, while the older marine groundwaters of the Littorina groundwater type show magnesium concentrations between 150 and 290 mg/L and are found at depths between 100 and 200 m (Figure 4-6a). The highest magnesium concentrations in the Forsmark site groundwaters (around 287 mg/L) are also found in the Littorina groundwater type present in the upper 200 m. Thus, from the upper 200 m in the SFR site, a range between 79 and 290 mg/L for magnesium could be proposed (Table 4-1 and Table 4-2).

Dissolved potassium concentrations

The potassium concentration in the SFR groundwaters ranges from 3.8 to 60 mg/L (Table 4-1, Figure 4-6c, d and Figure 4-10a, b). The contents are especially high in the two marine type groundwaters as shown by the two peaks in Figure 4-6d, at chloride concentrations close to 3,000 mg/L (local Baltic type), and at about 5,500 mg/L (Littorina type). However, compared with the groundwaters from the Forsmark site, none of the samples in the SFR dataset reflects the strongest Littorina signatures found there.

The highest variability and also the highest potassium contents (3.8 to 60 mg/L) found in the SFR groundwaters have been measured in the first 100 m depth, dominated by the Local Baltic type groundwaters (Figure 4-6c). In the Forsmark area the highest variability in this element (with a similar range, 4.9 to 67.8 mg/L; Figure 4-6c, d and Figure 4-10c, d), was also found at the same depth range though in this case the Littorina type dominated the groundwaters. A potassium range, from 3.8 to 60 mg/L (Table 4-1 and Table 4-2), has been selected here.

Dissolved silica concentrations

Silica concentrations in the SFR groundwaters range from 2.6 to 17.2 mg/L (Table 4-1 and Figure 4-10a, b), with the lowest values in one of the Local Baltic type groundwaters and the highest in some Local Baltic and Littorina type groundwaters (Figure 4-7a). However, more than 98% of the samples display silica contents between 7 and 14 mg/L (Figure 4-10a). This variability range decreases with depth in such a way that at 250 m depth, the silica contents range from 10 to 13 mg/L (Figure 4-7a).

Silica values in the SFR groundwaters are similar to the ones reported for other crystalline rock systems (e.g. Forsmark, Laxemar, Olkiluoto, Palmottu or the Lac du Bonnet granitic batholith in Canada) at levels shallower than 500 m depth[3] (Gimeno et al. 2009).

In the case of the groundwaters from Forsmark and Laxemar sites, this variability is frequently related to the variable seawater influence. For instance, the widest variability and highest silica contents in the Forsmark groundwaters (up to 24 mg/L; Figure 4-7a and Figure 4-10c, d) are related to the brackish groundwaters characterised by an important Littorina contribution, also displaying high and variable contents of dissolved sulphate, magnesium and manganese, inherited from their marine origin (Gimeno et al. 2008).

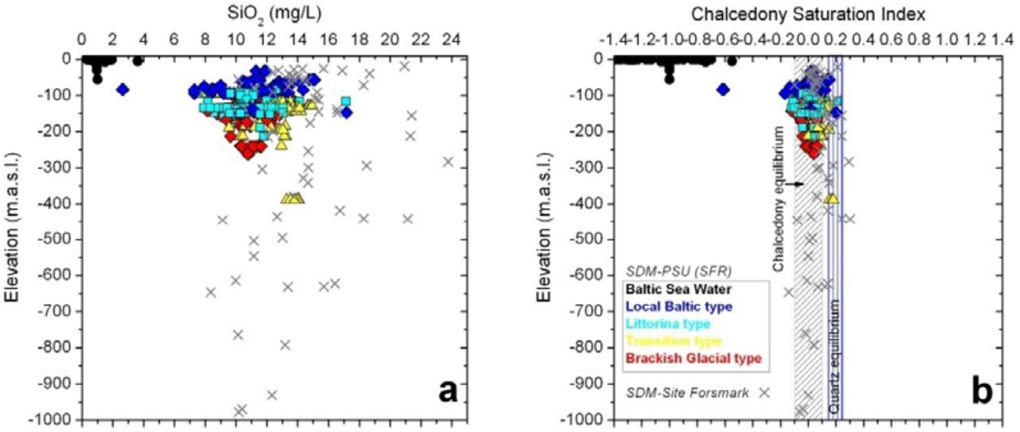

Figure 4-7. *Silica concentrations (a) and saturation index values for chalcedony (b) versus depth in the SFR. The diagrams show these data integrated in the general distribution of the Forsmark SDM groundwater data. Dashed areas in panel b correspond to the uncertainty ranges associated with the saturation indices calculations (see Gimeno et al. 2011 for further details).The SFR groundwater samples are colour coded according to the different groundwater types defined for the SFR Site by Nilsson et al. (2011).*

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[3] The silica values observed in the most saline (Cl > 7,000 mg/L) and deep groundwaters of these systems are relatively constant between 6.4 and 10.7 mg/L (Gimeno et al. 2009).

High silica concentrations can be acquired by marine waters when passing through sea-bottom sediments with highly soluble diatom skeletons (made of amorphous silica) and diatom ooze and diatomaceous muds are frequently present in the Littorina sediments (Burke and Kemp 2002 and references therein). As these silica rich recharge waters flow through the bedrock, silica concentrations would decrease by reaction with the fracture filling minerals, especially with clays (e.g. McKenzie et al. 1967). However, in the Forsmark site it is clear that these reactions have not been able to eliminate the high dissolved silica contents, which remain as a fingerprint of an old mixing process (the input of the Littorina waters).

In the Laxemar site the Littorina imprint on silica concentrations (and in general) seems to have been weaker and/or more easily removed (e.g. through sorption processes in fracture filling clays) as there is no clear relation between waters with high Littorina mixing proportion and high silica contents. However, the lowest contents of dissolved silica (4 mg/L) were found in some samples from KAS02 borehole (Äspö) at 307.68 m depth in groundwaters with an important contribution of present Baltic Sea waters (Glynn and Voss 1999, Gimeno et al. 2009) with depleted silica concentrations due to biological extraction (present Baltic Sea waters show very low silica contents, usually below 1 mg/L).

Thus, marine influences can promote the existence of both high and low dissolved silica contents depending on the heterogeneous reactions during the infiltration of seawaters through the marine sediments. In the SFR groundwaters, both types of marine influences are present. The two highest silica concentrations (around 17 mg/L) have been measured in Littorina type and Local Baltic type groundwaters, and the lowest silica concentrations are also associated with Local Baltic type groundwaters (HFM34 borehole at 83 m depth; Gimeno et al. 2011).

The hydrochemistry of these Local Baltic type groundwaters is almost identical to the Baltic Sea waters sampled at the SFR site (Gimeno et al. 2011) but with silica contents two or three times higher (around 2.6 mg/L). Therefore, these groundwaters from the HFM34 borehole would correspond to present Baltic Sea waters without any mixing with older groundwaters, but their higher silica contents would be derived from water-rock interaction processes, probably with clay minerals present in the fracture fillings.

Overall, most groundwaters in the SFR area would be at equilibrium or closer to equilibrium with chalcedony (or, alternatively, with quartz if the solubility data proposed by Rimstidt (1997[4]) are considered; see Gimeno et al. (2009) for further details) irrespective to their depth and salinity, in common with the Forsmark site (Figure 4-7b) and in other "similar" crystalline environments such as Olkiluoto or Lac du Bonnet (Gimeno et al. 2009). Only the recent Baltic groundwaters from the HFM34 borehole (together with present day Baltic Sea waters) are clearly undersaturated with respect to both phases, which suggests that water-rock interaction processes have not had either the time (i.e. Baltic waters are typically about 13.5 TU) or the necessary intensity to impose the dissolved silica contents found in other groundwaters (Gimeno et al. 2011).

Another observation is the slightly broader range of saturation indices in the shallower and less saline samples compared with the deeper and more saline groundwaters, both in the SFR and in the Forsmark sites (Figure 4-7b) and also in the Laxemar site groundwaters (Gimeno et al. 2009). This slightly greater dispersion in the chalcedony saturation index (SI) values in all these systems at shallow depths may be related to the superposition of other processes controlling the dissolved silica (e.g. aluminosilicate reactions and/or mixing processes such as the previously mentioned "disturbance" induced by the marine contributions). In these cases, dissolved silica concentrations might not be controlled by chalcedony equilibrium but by incongruent dissolution reactions or surface processes involving clay minerals in fracture fillings (see Gimeno et al. 2009 for further discussion).

Therefore, though the most frequent range found for the SiO_2 content in the SFR groundwaters is 7–14 mg/L, the recommendation is to consider a broader range, from 2.6 to 17.2 mg/L (Table 4-1 and Table 4-2), for the saline reference water.

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[4] The measurement of quartz solubility under low-temperature conditions (21 to 96°C) by Rimstidt (1997) indicates a considerably greater solubility ($\log K = -3.746$ or 11 ppm as SiO_2 at 25°C) than previously reported and generally accepted ($\log K = -4$ or 6 ppm of dissolved SiO_2). The experiments by Gunnarsson and Arnórsson (2000) seem to have confirmed the findings of Rimstidt (1997). See Gimeno et al. (2009) for further details.

Eh values

From the geoscientific investigation programme for the SFR extension project twelve Eh logs in seven borehole sections, from depths between 94 and 154 m, are available (Nilsson et al. 2011, Gimeno et al. 2011). The selection of the representative Eh (and pH) values for each specific borehole section from the SFR area has been based on a careful analysis of the data delivered by SKB database (SICADA) and on the data available in other reports (e.g. Lindquist and Nilsson 2010, Nilsson 2011). The whole selection procedure, similar to that used in the Site Characterisation Programmes from the Forsmark and Laxemar areas (Gimeno et al. 2008, 2009), is described in Gimeno et al. (2011).

Six of the twelve revised Eh values show a mildly reducing character whereas the rest indicate slightly oxidising conditions. The measured oxidising Eh values in the SFR groundwaters (from +30 to +110 mV) appear to be controlled by amorphous Fe(III)-oxyhydroxides and it is concluded that these oxidising conditions could be representative of groundwaters affected by some artefact (failures in the sealing capacity of the equipment) related to the oxic environment in the tunnels (Gimeno et al. 2011).

The sections with reducing values (from −140 to −190 mV; Figure 4-8) correspond to Littorina and Local Baltic-type groundwaters except the one with the most reducing value (−190 mV), which is a glacial-type groundwater from KFR105 (at −154 m.a.s.l.). These negative values are in line with the measured Eh values from the Forsmark site (mainly, those of Littorina type brackish marine groundwaters; Figure 4-8).

Redox potentials were also calculated from the redox couples (Gimeno et al. 2011) for the whole set of groundwater samples comprising suitable data. The selected redox couples are those of sulphur and iron (including the Fe^{3+}-clay/ Fe^{2+}-clay redox pair; see Nilsson et al. 2011 and Gimeno et al. 2011), which have provided meaningful results in this and in previous studies. Calculations have been performed with both the measured pH values and the ones calculated in equilibrium with calcite and the results are presented in Figure 4-9.

Sulphur redox pairs would provide reducing values for the SFR groundwaters. Values from the SO_4^{2-}/HS^- and SO_4^{2-}/FeS_{am} redox couples, which have generally shown a good agreement with the potentiometrically measured Eh values in the Site Investigations (Gimeno et al. 2008, 2009), would be around −200 mV. The Fe^{3+}-clay/ Fe^{2+}-clay redox pair would lead to less reducing values (mean around −120 mV).

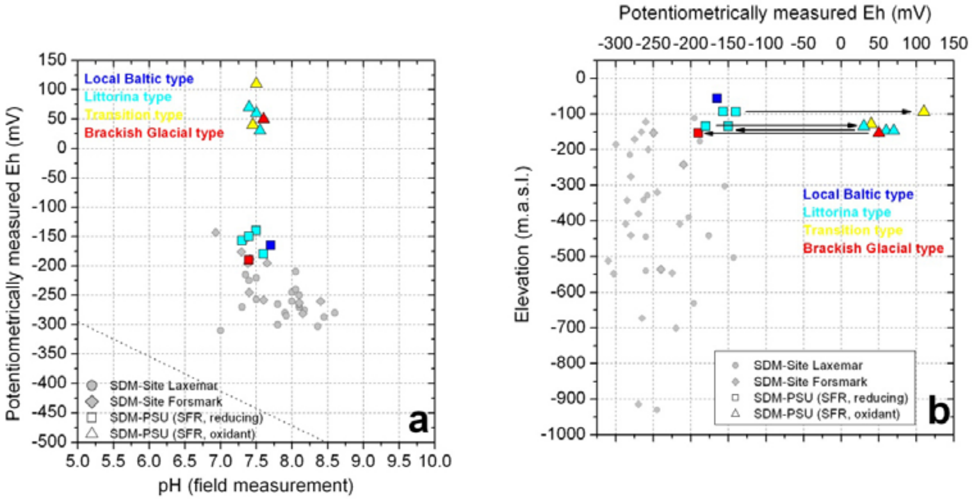

Figure 4-8. *Potentiometrically measured Eh values versus pH (a) and depth (b) for the SFR and the Forsmark and Laxemar SDM groundwaters. SFR values are colour coded as in the previous figures. Arrows in panel b indicate the shift observed in the Eh value with time in some of the samples.*

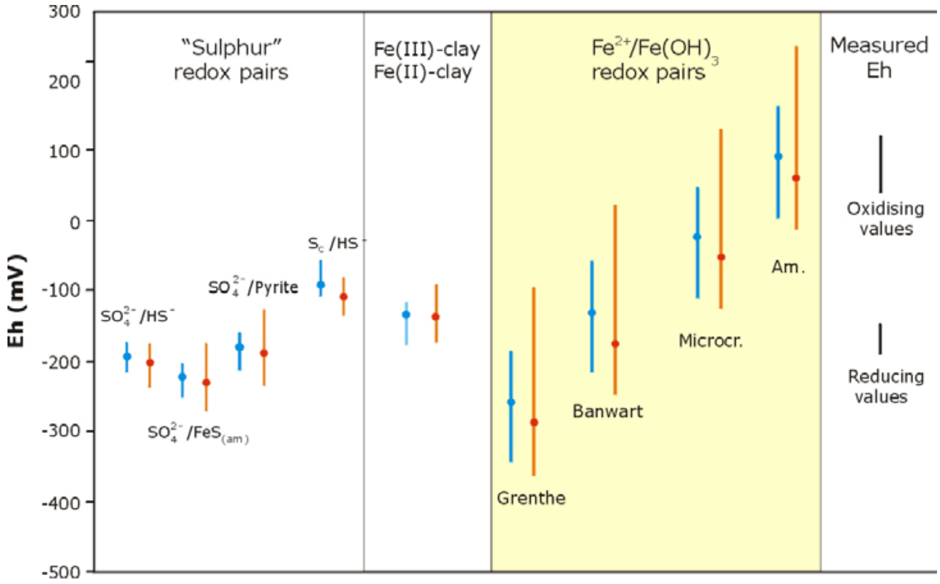

Figure 4-9. *Eh values calculated from different redox couples for the whole suitable set of SFR groundwaters, compared with the potentiometrically measured Eh values. Red lines represent the range of values obtained with the measured pH and blue lines the range of Eh values obtained with the calculated pH. Circles represent the mean value for each case. Taken from Gimeno et al.(2011).*

From the scarce data available for methane (four samples) values for the CO_2/CH_4 redox pair can be obtained. Redox potential results for this pair are very similar to the ones obtained with the sulphur couples (from −208 to −233 mV) even taking into account the possible impact of pH uncertainty on the calculated values (11 mV of Eh uncertainty in the worst case). A similar agreement has also been reported for the Forsmark and the Laxemar SDM groundwaters (Gimeno et al. 2008, 2009).

The redox potential defined by the $Fe^{2+}/Fe(OH)_3$ heterogeneous redox pair depends on the mineral phase characters (solubility, particle size, etc.) of the specific ferric oxyhydroxide included in the calculations. For a crystalline Fe(III)-oxyhydroxide (like hematite, frequently found in the facture fillings of the SFR), the results obtained using the Grenthe's solubility value (Grenthe et al. 1992) would be between −100 and −350 mV. Only the calculations considering microcrystalline or amorphous phases, representative of oxic or post-oxic environments, provide oxidising values.

Overall, most of the selected redox pairs suggest the existence of reducing Eh values for the SFR groundwaters in accordance with the chemistry of Fe, Mn, S and U (Nilsson et al. 2011, Gimeno et al. 2011). For sulphidic and methanic groundwaters, Eh values between −200 and −220 mV could be proposed. For the rest, values below −100 mV could be feasible considering the redox couples usually active in the studied systems. Thus, taking into account measured and calculated redox potentialas, an overall range from –100 to –350 mV (Figure 4-10f and Table 4-1 and Table 4-2) could be proposed for the Eh values in the SFR groundwaters.

This range agrees very well with what has been obtained from the Site Characterisation Programmes of the Forsmark and Laxemar areas. Eh values measured at Forsmark site at depths between 100 and 900 m (Gimeno et al. 2008) are between −143 and −281 mV (Figure 4-8), while in the Laxemar area they are more reducing, between –200 and –310 mV (Figure 4-8) (Gimeno et al. 2008, 2009).

Overall, the distribution of Eh values with depth (Figure 4-8b) does not show any evident trend in these systems but they are clearly reducing (lower than −150 mV) below 100 m depth in Forsmark and Laxemar sites (apart from the values measured in SFR, there are no other Chemmac measurements at shallower depths). Therefore, from the values measured in these two sites, a range of Eh between −143 and −310 mV could be suggested, similar to the range proposed for the SFR system (Table 4-2).

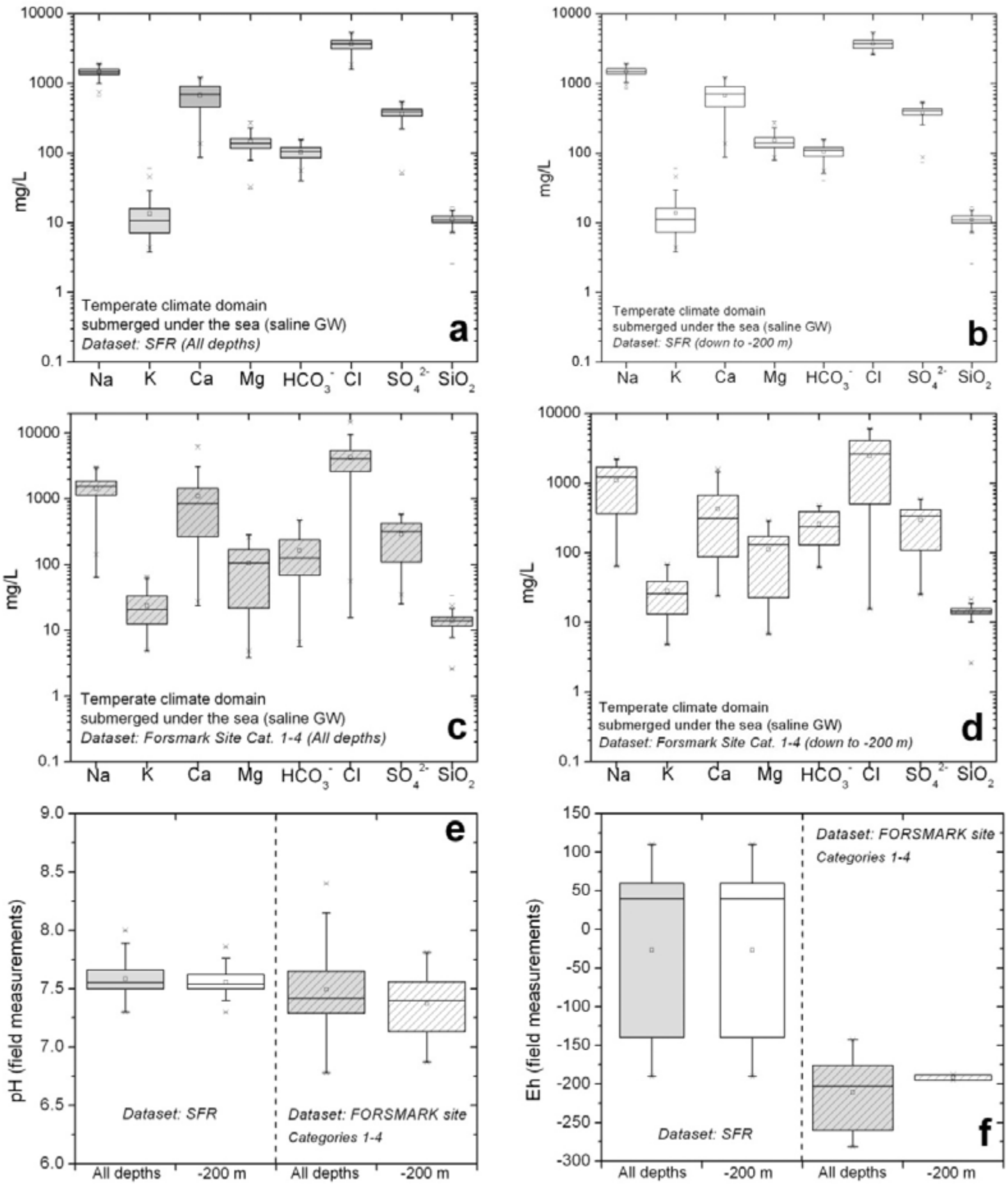

***Figure 4-10.** Box-and-whisker plots showing the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the SFR for the whole set of samples (a) and for the samples located in the first 200 m depth (b). Figures c and d show the same kind of information considering the Forsmark site groundwater samples as a comparative term; only samples from categories 1 to 4, as defined in the SDM (Laaksoharju et al. 2008) have been considered. Figure e and f show the values corresponding to pH and Eh for the different datasets. The statistical measures plotted here and in all the following box and whiskers plots, are the median (horizontal line inside the grey box), the 25th and 75th percentiles (bottom and top of the box), the mean (square), the 5th and 95th percentiles ("whiskers"), the 1st and 99th percentile (crosses) and the maximum and the minimum values (horizontal bars).*

Discussion and conclusions

Table 4-2 summarises the concentration ranges for the different components in the SFR groundwaters. According to the previous description, two possible ranges have been defined depending on the dataset used (all samples or only the samples located down to –200 m depth). A possible composition for the reference water for this period is given, whose values are inside any of the two ranges indicated above. This water is slightly more dilute (calculated TDS = 6.26 g/L) than those proposed in previous safety assessments (TDS = 8.91 g/L for the SFR-1, SKB 2008a, and 9.49 g/L for the previous one in Wikberg (1999); Table 4-2). This TDS decrease is basically associated with its lower contents in chloride, sulphate, sodium and magnesium.

Maximum dissolved chloride contents present in the SFR groundwaters are some what lower than the ones considered previously in other assessments (5,500 vs. 6,000 mg/L; Table 4-2). Additionally, most groundwaters show chloride contents between 2,800 and 4,500 mg/L andthere are very few waters close to 5,500 mg/L Cl (Figure 4-1a). Therefore, to consider chloride contents more similar to the observed range seems to be more reasonable.

Values proposed for sulphate and magnesium in previous assessments correspond to the maximum values of the ranges observed in the SFR groundwaters. Most groundwaters show magnesium contents between 100 and 200 mg/L (Figure 4-10a, b) and have sulphate contents lower than 400 mg/L (Figure 4-10a, b). This situation is more exaggerated for sodium as the values proposed in the previous assessments (2,500 mg/L) are even higher than those observed in the SFR groundwaters (with maximum values of 1,900 mg/L; Figure 4-10a, b, Table 4-1 and Table 4-2). All this suggests the need to decrease the values considered for these components with respect to those proposed previously.

Calcium contents were also quite different in the previous assessments, 430 mg/L in SFR-1 and 1,000 mg/L in the previous one (Wikberg 1999; Table 4-2). The value suggested here (600 mg/L) is in between them and would correspond to the values of the SFR groundwaters at present, with the chloride contents selected for the reference water.

However, SiO_2 contents are higher than those proposed in the previous SFR-1, where they were calculated assuming that the proposed groundwater was in equilibrium with quartz (Höglund 2001, SKB 2008a). Here we have indicated that the dissolved silica content in the analysed groundwaters shows, in many cases, the fingerprints of mixing processes with marine waters and therefore, it mightn't necessarily be controlled by a silica phase. Moreover, had these waters been in equilibrium with one of these phases, it would have been chalcedony or the "new" quartz whose solubility data was proposed by Rimstidt (1997). Thus, some higher values, like those suggested in the present assessment, would be expectable.

The redox potential defined by the $Fe^{2+}/Fe(OH)_3$ heterogeneous redox pair depends on the mineral phase characters (solubility, particle size, etc.) of the specific ferric oxyhydroxide included in the calculations. For a crystalline Fe(III)-oxyhydroxide (like hematite, frequently found in the facture fillings of the SFR), the results obtained using the Grenthes solubility value (Grenthe et al. 1992) would be between −100 and −350 mV. Only the calculations considering microcrystalline or amorphous phases, representative of oxic or post-oxic environments, provide oxidising values.

The proposed composition for the reference groundwater (Table 4-2) has been obtained by expert judgement based on the statistical distribution of the values but slightly rounded to get a good electrical balance. This procedure has been followed for the rest of the proposed compositions. The percent error in the electrical balance is 0.27% and the composition is in equilibrium or near to equilibrium with calcite (SI = +0.03) and quartz[5] (SI = +0.15, using the solubility data proposed by Rimstidt (1997). Overall, as indicated above, the proposed values for the different parameters (except those for Eh) are near the mean and median values presently found in the SFR groundwaters (see Table 4-1).

4.1.2 Temperate climate domain with the repository above the sea level

During this domain, the climate will still be temperate but, due to isostatic uplift, the repository will not longer be beneath the sea. In the previous assessment (SKB 2008a) it was estimated that the shoreline would pass over the SFR approximately 1,000 years after closure. As a result, the flow pattern and the local groundwater system will evolve towards a steady-state situation, controlled by the local topography and, therefore, the origin and chemical composition of the water that reaches the silo repository and the rock vaults will change.When the local groundwater system has reached a steady-state situation, shoreline displacement will no longer affect the local situation at SFR, since the shoreline will then be far away.

Under these circumstances, the water will change to a young fresh groundwater (with a low chloride content) originated from recharge areas (above the sea level, inland) near the repository. Thus, it is assumed that the groundwater flowing into the repository will be fresh (non-saline) throughout this period.

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[5] Saturation index calculations have been performed at 15°C.

In the previous assessment, the composition of this fresh groundwater was assumed to be similar to that found in wells in Östhammar Municipality at present (Höglund 2001, SKB 2008a). The proposed value for potassium and its variation interval wasbased on general measurements made by SGU in Sweden ("SGUs grundvattennät" and "PMK-grundvatten") and on the proposed values for a standard water (Bertills 1995, Höglund et al. 1997) that are based on observed concentrations in deep groundwaters in igneous rock (Höglund 2001).

The dataset used in the present assessment for the selection of the reference water for this period, was collected from groundwaters exclusively derived from meteoric recharge. These data comprise the available data from the SDM investigations (Tröjbom and Söderbäck 2006a, b, Gimeno et al. 2008, 2009, Laaksoharju et al. 2008, 2009) on the fresh near-surface groundwaters and on the fresh shallow groundwaters from the Forsmark and Laxemar SDM areas.The near-surface groundwaters (NSGW) correspond to samples taken from soil tubes in the overburden at < 20 m depth from ground surface, whereas the shallow groundwaters correspond to samples taken in the percussion boreholes between 20 to100 m depth from ground surface. In both cases the only groundwaters selected for this climate period from the whole group are those with chloride contents lower than 500 mg/L and that is why they are called "fresh". In the near-surface dataset, waters with chloride content higher than 500 mg/L are associated with marine influence or influence of older and more saline discharge waters (Tröjbom and Söderbäck 2006a, b, Gimeno et al. 2008, 2009), and in the shallow groundwaters dataset, waters with chloride content higher than 500 mg/L are those affected by mixing with older and more saline waters (Gimeno et al. 2008, 2009). These groundwaters have been removed from the fresh near surface and shallow groundwaters datasets used for this climate domain.

Additionally, the set of water samples taken in the area of Uppland have also been considered for comparison only considering the fresh near surface and shallow groundwaters. The main difference with respect to the Forsmark and Laxemar sites groundwaters is that the Uppland ones have not undergone a categorisation process. Despite the big number of samples available for the Uppland dataset, only a few of them have been analysed for all the main components and these are the ones that have been considered here, 35 samples for the fresh near surface groundwater set (much smaller than for Forsmark or Laxemar datasets) and 75 for the fresh shallow groundwater set (larger than the datasets for the other two areas).

There is not hydrochemical information available on the SFR area to be used in this case as the repository is under the seafloor at present and no significant evidence of meteoric recharge waters has been found. Therefore, the data from the Forsmark site can be considered the most suitable for this assessment due to its proximity to the SFR. However, in the case of a very long temperate period (as in the *"extended global warming climate case"*), the SFR area would remain as a more hydraulically active recharge system as it has occured in Laxemar. Under these conditions, fresh groundwaters are expected to extend to greater depths and, depending on the length of the period, the calcite content in the overburden will also decrease to levels similar to the ones present in Laxemar. Therefore, Laxemar groundwater data can be used to put the estimations based on the Forsmark site data, into a broader context.

Finally, even taking into consideration the chemical characters of the near-surface groundwaters (as analogues for the recharge water over this period), compositional features of the shallow fresh groundwaters look more appropriate as analogues to the waters expected to be at the SFR repository depth during this climatic domain and they will be the basis for the final composition of this reference water.

Dissolved chloride concentrations

Dissolved chloride contents in the near-surface groundwaters from Forsmark and Laxemar sites show a wide variation (from 3.9 to 3,800 mg/L and from 3.2 to 3,900 mg/L, respectively). The high values are scarce and correspond to groundwaters affected by relict or modern marine inputs. However, most of the near-surface groundwaters show chloride contents below 200 mg/L in Laxemar and below 500 mg/L in Forsmark (Tröjbom and Söderback 2006a, b, Gimeno et al. 2008, 2009). Shallow groundwaters in the Forsmark site also display a wide variability in chloride and generally fall within the category of mixed brackish groundwaters, due partly to the mixing of discharging brackish marine (Littorina) groundwaters (and/or residual near-surface brackish-saline waters of Baltic Sea origin) with recharging meteoric waters. In the footwall bedrock segment (including fracture domains FFM01 and FFM02; Laaksoharju et al. 2008), this shallow system is controlled by flow along highly transmissive, well-connected system of sub-horizontal fractures (i.e. the shallow bedrock aquifer), which is still in the process of flushing out residual brackish marine (Littorina) groundwaters. This also produces a mixing effect between recharging meteoric waters and residual brackish (possibly including Baltic Sea) groundwaters (Laaksoharju et al. 2008).

However, considering only the fresh shallow groundwaters, the ranges are narrower. They show chloride contents between 15.7 and 503 mg/L in the Forsmark site groundwaters (Figure 4-11b and Table 4-3) and in the case of Laxemar, between 6 and 357 mg/L (Figure 4-11d and Table 4-3). For the Uppland set of samples, the contents range between 3.2 and 365 mg/L (Figure 4-11f and Table 4-3). Thus, the wider range found in the fresh shallow groundwaters from the Forsmark SDM (15.7–503 mg/L) are proposed for the reference fresh groundwaters expected around the repository, when not submerged under the sea, during the temperate climate domain (Table 4-5).

Dissolved sulphate concentrations

Dissolved sulphate contents in the whole set of near-surface groundwaters from the Forsmark site range from 0.7 to 387 mg/L (Tröjbom and Söderbäck 2006a). The highest concentrations are associated with soil pipes with a clear marine contribution (chloride contents near 4,000 mg/L) whereas the fresh near-surface groundwaters show dissolved sulphate concentrations lower than 251 mg/L (Table 4-3).

Something similar has been found in the Laxemar-Simpevarp near-surface groundwaters where the fresh-type shows dissolved sulphate contents between 0.8 and 176 mg/L (Figure 4-11c and Table 4-3; Gimeno et al. 2008, 2009). The set of fresh near-surface groundwaters from the Uppland area show a slightly narrower range from 7.2 to 83.9 mg/L, although the small number of samples compared with the other sets could be the reason for this.

Fresh shallow groundwaters at Forsmark and Laxemar sites also show similar contents though the highest values are lower and the range narrower (25 to 163 mg/L in Forsmark and 17 to 110 mg/L in Laxemar, Table 4-3) than what was observed in their respective near-surface groundwaters. The case of the Uppland shallow groundwaters is just the opposite with values between 7.9 and 187 mg/L (probably due to the higher number of samples) higher and broader than in the near-surface groundwaters, but closer to what has been found in the same type of waters from the Forsmark site (Figure 4-11b and f). Therefore, values from the shallow groundwaters from the Forsmark SDM have been selected for the reference groundwater corresponding to this climate domain.

Dissolved sulphate contents in the near-surface groundwaters from Forsmark and Laxemar sites are controlled by the existence of multiple sulphur sources (e.g. atmospheric sulphur deposition, oxidation of sulphides) and by sulphate reduction processes (presumably the same could be applied to the Uppland area). In the fresh, shallow-groundwaters, the inherited dissolved sulphate contents from the recharge seem to be only modified by sulphate reduction processes as there is not any important solubility limiting phase for those groundwaters (mixing is the main control of dissolved sulphate in the brackish saline groundwaters from both sites; Laaksoharju et al. 2008, Gimeno et al. 2008, 2009).

Carbonate system: pH, calcium and alkalinity

pH values, in the near-surface groundwaters from the Forsmark site, range from 6.6 to 7.9 (Figure 4-11g and Table 4-3) and are lower than some values found in the deeper groundwaters (Laaksoharju et al. 2008). Similarly, calcium concentrations in those groundwaters are not as high as in some deeper groundwaters and most values are below 200 mg/L with a range between 29 and 232 mg/L (though they may reach values around 700 mg/l in some near surface saline waters, with Cl around 2,000 mg/L from soil tubes located in till under the sediments of lakes or under the sea; Tröjbom and Söderbäck 2006a).

Table 4-3. Statistical values for the fresh waters (Cl < 500 mg/L) taken near the surface (down to –20 m depth at the most) in the Forsmark site (Set a), Laxemar site (Set b) and the whole area of Uppland (Set c) and the fresh shallow groundwaters (down to –100 m depth) in the three areas (Sets d, e and f, respectively). These groups of waters have been used to select the reference Fresh Groundwater for the Temperate climate domain when the repository is not submerged under the sea.

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set a (Fresh NSGW Forsmark SDM)										
pH	147	7.09	0.24	6.6	7.07	7.9	6.6	6.73	7.55	7.9
Na	229	66.37	95.01	4.6	24.3	500	4.6	5.8	283	500
K	229	9.16	7.24	1.56	5.92	37.6	1.56	2.23	26.5	37.6
Ca	229	108.25	35.22	29	110	232	29	39.7	169	232
Mg	229	16.59	13.79	4.15	10.6	63.2	4.15	4.88	50.4	63.2
HCO_3^-	229	392.49	111.61	179	374	777	179	229	615	777
Cl	229	80.24	114.82	3.9	31.5	503.3	3.9	6.6	370	503.3
SO_4^{2-}	228	60.04	53.36	0.7	43.6	251.1	0.7	3.2	178.0	251.1
SiO_2	229	13.74	4.29	2.2	13.3	30.0	2.2	7.3	20.7	30.0
Set b (Fresh NSGW Laxemar SDM)										
pH	60	7.47	0.42	6.35	7.465	8.57	6.35	6.8	8.135	8.57
Na	137	48.87	58.86	4	28.8	249	4	4.9	213	249
K	137	5.74	7.23	0.97	4.01	46.3	0.97	1.13	13.5	46.3
Ca	137	41.75	22.99	2.7	39.7	104	2.7	9.1	81.3	104
Mg	137	9.66	8.29	0.88	8.1	45.2	0.88	2.29	28.8	45.2
HCO_3–	137	160.73	110.76	2.15	160	552	2.15	20.2	301	552
Cl	137	46.14	62.19	3.2	16.1	424	3.2	4	147	424
SO_4^{2-}	137	48.86	39.24	0.8	38.9	176.2	0.8	7.8	139.6	176.2
SiO_2	137	25.58	10.60	9.1	22.7	72.5	9.1	13.6	44.3	72.5
Set c (Fresh NSGW Uppland)										
Na	35	17.03	41.92	1.8	8.2	255	1.8	3	34	255
K	35	9.42	11.91	0.9	5.2	42	0.9	1	41	42
Ca	32	71.25	29.60	22	72	142	22	23	126	142
Mg	35	5.81	3.23	1.4	4.8	13	1.4	1.6	13	13
HCO_3^-	35	219.63	96.88	32	219	497	32	72	380	497
Cl	35	24.35	52.72	0.3	12.0	315.0	0.3	1.7	72.0	315.0
SO_4^{2-}	35	24.77	15.63	7.2	23.0	83.9	7.2	7.9	49.9	83.9
Set d (Fresh Shallow GW Forsmark SDM)										
pH	9	7.51	0.27	7.07	7.58	7.81	7.07	7.07	7.81	7.81
Na	19	251.82	89.69	64.6	256	399	64.6	64.6	399	399
K	19	9.63	3.46	5.6	9.32	15.3	5.6	5.6	15.3	15.3
Ca	19	49.72	23.24	23.9	41.1	102	23.9	23.9	102	102
Mg	19	12.80	6.03	6.91	9.01	23.4	6.91	6.91	23.4	23.4
HCO_3^-	19	420.89	43.65	310	446	473	310	310	473	473
Cl	19	218.12	154.46	15.7	184	503	15.7	15.7	503	503
SO_4^{2-}	19	86.73	33.61	25.3	94.7	163.0	25.3	25.3	163.0	163.0
SiO_2	19	15.63	2.16	13.3	14.6	20.9	13.3	13.3	20.9	20.9
Set e (Fresh Shallow GW Laxemar SDM)										
pH	0	–	–	–	–	–	–	–	–	–
Na	27	120.49	53.02	38.4	110	248	38.4	41.7	217	248
K	27	3.33	0.96	1.77	3.17	5.35	1.77	2	5.32	5.35
Ca	27	22.47	12.61	7.5	17	48.3	7.5	9.6	46.4	48.3
Mg	27	4.60	2.35	1.9	4.09	12.9	1.9	2.23	8.32	12.9
HCO_3^-	27	230.04	44.05	121	224	324	121	157	311	324
Cl	27	68.88	77.60	5.8	43.6	357	5.8	8.2	203	357
SO_4^{2-}	27	47.83	23.06	17.0	49.1	109.6	17.0	20.8	99.2	109.6
SiO_2	24	15.66	3.77	12.6	14.8	31.2	12.6	12.8	20.7	31.2
Set f (Fresh Shallow GW Uppland)										
Na	72	68.71	58.02	3.4	62.5	285	3.4	4.4	163	285
K	72	8.04	9.99	1.2	4.25	51	1.2	1.5	32	51
Ca	67	65.40	39.99	9.6	62	197	9.6	14	139	197
Mg	72	6.20	2.97	0.97	6.25	14	0.97	1.6	11	14
HCO_3^-	71	282.07	71.68	113	285	463	113	140	388	463
Cl	72	51.89	71.48	3.2	20	365	3.2	5.5	184	365
SO_4^{2-}	72	34.51	34.48	7.9	25.5	187.7	7.9	9.8	106.9	187.7

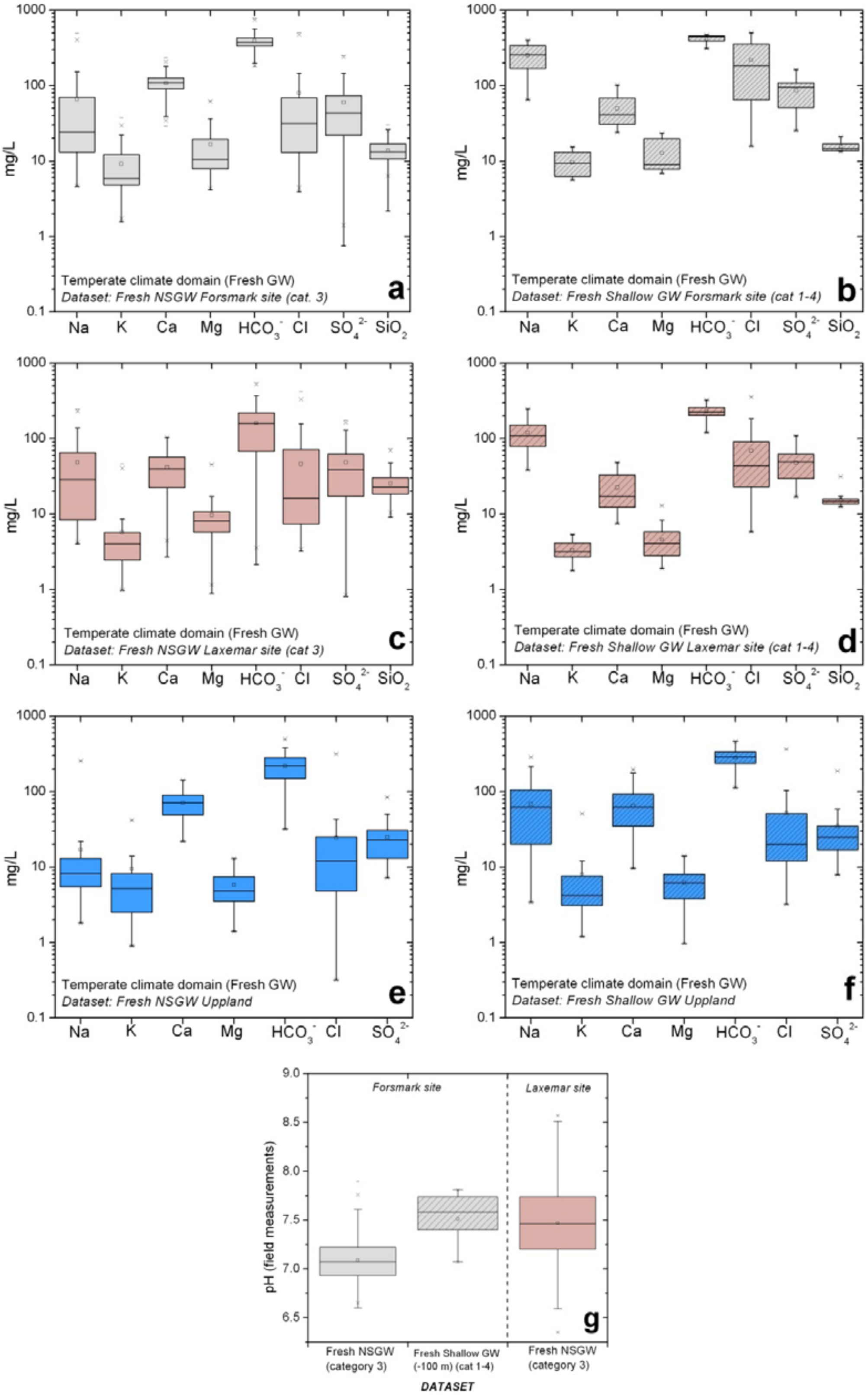

Figure 4-11. *Box-and-whisker plots showing the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the Fresh Near Surface Groundwaters from the Forsmark site (a; only category 3 samples), Laxemar site (c; only category 3 samples) and Uppland (e) and in the Fresh Shallow Groundwaters of the three places (b, d and f, respectively; only samples from categories 1 to 4, as defined in the SDM (Laaksoharju et al. 2008) have been considered for Forsmark and Laxemar datasets). Pannel g shows the values corresponding to pH for the Forsmark site groundwater samples included in panels a and b, and for the Fresh NSGW of the Laxemar site (in panel c) as a comparative term. See the caption of Figure 4-10 for the statistical meaning of the different symbols.*

Alkalinity (HCO_3^-) values show the widest variability and the highest values (from 40 to near 800 mg/L) in the whole set of near-surface groundwaters, mainly due to the influence of atmospheric and biogenic CO_2 and to the progress of carbonate and silicate weathering reactions in the overburden (Gimeno et al. 2008). In the group of fresh near-surface groundwaters, alkalinity (HCO_3^-) values range from 179 to 777 mg/L and in most cases from 179 to 500 mg/L HCO_3^- (Figure 4-11a, Table 4-3).

The extensive presence of limestones in the overburden of the Forsmark area (a feature very uncommon in the Swedish soils; Tröjbom and Söderback 2006a, Gimeno et al. 2008, 2009) promotes important differences in pH, alkalinity, calcium contents and calcite saturation indices in the near-surface groundwaters with respect to other investigated sites (e.g. Laxemar; Gimeno et al. 2008, 2009) and, in general, with respect to most excavated wells in Sweden (Tröjbom and Söderbäck 2006a). The range for the available field pH data in the fresh near-surface groundwaters do not show clear differences between the two areas, although lower values, as a whole, appear to occur in Forsmark (Figure 4-11g). Calcium and bicarbonate contents are clearly lower in the Laxemar site groundwaters (Figure 4-11a and c) and undersaturation states with respect to calcite are much more frequent in this zone.

There are no pH measurements in the near-surface groundwater data from the Uppland area. Calcium contents show values from 22 to 142 mg/L (intermediate between the values found in the same type of waters in Forsmark and Laxemar sites) and alkalinity ranges from 32 to 497 mg/L (slightly lower than in the other two areas, probably because of the smaller number of samples; Figure 4-11e and Table 4-3).

Fresh shallow groundwaters in the Forsmark site (< 100 m depth and Cl < 500 mg/L) are characterised by narrower ranges in the examined parameters, than the fresh near-surface groundwaters of this area (Figure 4-11a and b): calcium and bicarbonate contents range from 24 to 102 mg/L and from 310 to 473 mg/L, respectively; pH values range from 7.0 to 7.81 and, mostly, from 7.3 to 7.8; Figure 4-11g, Table 4-3). Fresh shallow groundwaters in Laxemar show even narrower ranges and lower values than in the Forsmark site groundwaters (7.5 to 48.3 mg/L Ca and 121 to 324 mg/L HCO_3^-; Figure 4-11d; *in situ* pH measurements are not available; Table 4-3). As for the rest of the elements, the larger number of fresh shallow groundwaters from Uppland gives broader ranges for calcium and alkalinity, from 10 to 197 mg/L and 113 to 463 mg/L, respectively (Figure 4-11f and Table 4-3).

Overall, the unusual features of the overburden in Forsmark SDM area (compared with other Swedish sites) condition the chemical character of the near-surface groundwaters and eventually the chemistry of the fresh shallow groundwaters. This is why these waters are clearly different from other sites such as Laxemar. Thus, values from the shallow groundwaters from Forsmark SDM dataset can be selected for dissolved calcium and alkalinity of the reference fresh water during the temperate climate domain when the repository is not covered by the sea. For the specific case of an *"extended global warming*", Laxemar ranges would be more suitable over time.

Biogenic CO_2 inputs and weathering reactions control the evolution of the carbonate system (and related concentrations) in the overburden. But, also, calcite participates in the regulation of alkalinity and dissolved calcium as solubility limiting phase. This mineralogical control persists in the shallow groundwaters which are, usually, in equilibrium with respect to this mineral (Gimeno et al. 2008, 2009).

Dissolved magnesium concentrations

Magnesium contents in the near-surface groundwaters from the Forsmark site range from 4.15 to 179 mg/L, with the highest values in the waters with a clear marine contribution. Overall, 90% of the near-surface groundwaters show contents lower than 85 mg/L Mg (Tröjbom and Söderbäck 2006a, b) and most of the fresh near-surface groundwaters have contents lower than 63 mg/L (Figure 4-11a, Table 4-3). Something similar has been found in the Laxemar site, where the marine influence gives magnesium contents up to 350 mg/L in some near-surface groundwaters; while the fresh waters only reach values lower than 45.2 mg/L (Figure 4-11c, Table 4-3).

Dissolved magnesium contents in the fresh shallow groundwaters from the uppermost zone in the bedrock of both areas, are even narrower: below 23.4 mg/L Mg in the Forsmark site dataset and lower than 13 mg/L Mg in Laxemar (Figure 4-11b and d, Table 4-3). The values found in both, the fresh near surface and shallow groundwaters from the Uppland area, are low, ranging from 0.9 to 14 mg/L.

Therefore, a range of 7 to 24 mg/L for dissolved magnesium can be proposed from the shallow groundwaters from the Forsmark site.

Magnesium contents in the fresh near-surface groundwaters from these sites are mainly controlled by aluminosilicate weathering reactions, although marine contributions may play a role even in these fresh groundwaters of the overburden (Tröjbom and Söderbäck 2006a, b, Gimeno et al. 2008, 2009). Deeper, in the bedrock, mixing processes are the main control on dissolved magnesium concentrations in brackish and saline groundwaters (even considering the reactive character of this component) and this element is considered a tracer of marine signatures (Laaksoharju et al. 2008, Gimeno et al. 2008, 2009).

Dissolved magnesium in the fresh, "recently" recharged groundwaters must be controlled by water-rock interaction processes (e.g. dissolution-precipitation or cation exchange processes involving chlorite and mixed-layer clays like smectite/ illite, chlorite/smectite or chlorite/vermiculite, frequently found in the fracture fillings (Gimeno et al. 2008, 2009).

Dissolved sodium concentrations

Sodium concentrations in the near-surface groundwaters from the Forsmark site range from 1 to 1,600 mg/L. Similar to magnesium, the higher values correspond to groundwaters with a clear marine influence. More than 75% of the whole set of near-surface groundwaters show sodium contents lower than 500 mg/L, the same as in the subset of fresh near-surface groundwaters (Figure 4-11a, b, Table 4-3). The highest sodium contents dissolved in the near-surface groundwaters of Laxemar reach values between 1,900 and 2,230 mg/L and they correspond to waters influenced by marine signatures and by discharging deep groundwaters (Gimeno et al. 2009). However, as in Forsmark, fresh near-surface groundwaters show much lower contents, below 213 mg/L and in most cases, below 125 mg/L (Figure 4-11c, Table 4-3). The same maximum values have been observed in the fresh near-surface groundwaters from Uppland (Na < 255 mg/L). Low values in sodium concentrations have also been found in the fresh shallow groundwaters from the three areas: 64.6 to 399 mg/L in the Forsmark site, 38.4 to 248 mg/L Na in the Laxemar site and 3.4 to 285 mg/L in the Uppland area (Figure 4-11b, d and f, Table 4-3) Therefore, the range found in the shallow groundwaters from the Forsmark site has been selected for the reference fresh waters around the repository when not submerged under the sea during the temperate climate domain.

In common with magnesium, weathering reactions and water-rock interaction processes are involved in the control of dissolved sodium in the fresh groundwaters of the overburden and the shallow bedrock (Gimeno et al. 2009).

Dissolved potassium concentrations

As for magnesium and sodium, dissolved contents of potassium show a wide variability in the near-surface groundwaters from the Forsmark and Laxemar SDM areas (from 1.8 to 70 mg/L and from 1–94 mg/L, respectively) with the highest values associated with marine contributions. Fresh near-surface groundwaters of both zones show lower values, mostly below 37 mg/L K in Forsmark SDM dataset and below 46.3 mg/L K in Laxemar SDM dataset (Figure 4-11a, c and Table 4-3). The values in the Uppland fresh near-surface groundwaters are similar, all below 42 mg/L (Figure 4-11e, Table 4-3).In the fresh shallow groundwaters from Forsmark and Laxemar sites, dissolved potassium contents are even lower, from 5.6 to 15.3 mg/L in Forsmark and from 1.8 to 5.3 mg/L in Laxemar (Figure 4-11b, d andTable 4-3). However, potassium content in the fresh shallow groundwaters from Uppland show a broader range (from 1.2 to 51 mg/L) similar to what is found in the near-surface groundwaters (Figure 4-11e, f and Table 4-3).

Values from the shallow groundwaters in the Forsmark SDM dataset have been selected for the reference water.

As indicated above for magnesium and sodium, dissolved potassium may be partially controlled by mixing in the brackish and saline groundwaters in the bedrock. However, weathering reactions and water-rock interactions (reaction with aluminosilicates, or cation-exchange) control the behaviour of this element in the near surface and shallow groundwaters (see Gimeno et al. 2008, 2009 for further details).

Dissolved SiO_2 concentrations

Fresh near-surface groundwaters in the Forsmark site show a large variability in silica contents although they are usually lower than 30 mg/L (Figure 4-11a, Table 4-3). Fresh near-surface groundwaters from the overburden of similar systems (Laxemar, Olkiluoto and the Canadian Shield) also have a large variability (and some very high silica contents). The maximum silica concentrations in near-surface groundwaters from Laxemar reach 72.5 mg/L, although they are usually lower than 45 mg/L (Figure 4-11c, Table 4-3). Near-surface groundwaters in Palmottu and in the Canadian Shield reach values of 30 mg/L and 24 mg/L, respectively, and groundwaters from the overburden in Olkiluoto peak at 25 mg/L but they are usually below 15 mg/L (Gimeno et al. 2009). These large variations are associated with the local presence of easily alterable silica phases and/or with the intensity of weathering reactions in the overburden.

Silica contents in the fresh shallow groundwater (FSG, < 100 m depth) from the Forsmark site show a narrower range (between 13.3 and 20.9 mg/L; Figure 4-11a, Table 4-3) in common with the aforementioned systems (e.g. 12.6 to 31.2 mg/L in Laxemar; Figure 4-11c, Table 4-3). There are not silica data for the Uppland groundwaters.

Silica contents in the near-surface groundwaters from these sites are mainly controlled by aluminosilicate weathering reactions: silica released from primary minerals is partially incorporated into secondary clays and the net effect on the concentration of dissolved silica depends on the type of secondary mineral phase. Quartz and/or chalcedony are not involved as a limiting solubility phase in the control of dissolved silica as near-surface groundwaters are frequently oversaturated with respect to both phases (Gimeno et al. 2008, 2009).

Deeper groundwaters, including the fresh groundwaters of meteoric origin at very shallow depths (<100 m depth; that is the fresh shallow groundwaters), are in equilibrium or near equilibrium (within the considered uncertainty range of ± 0.25 SI units; Gimeno et al. 2008) with respect to chalcedony or other silica variety with similar solubility (e.g. quartz with the "new" solubility data proposed by Rimstidt (1997), see Gimeno et al. (2009) for further discussion). However, those silica phases may not necessarily represent the minerals controlling dissolved silica concentrations, especially in dilute groundwaters. Feldspars and clay minerals in fracture fillings are probably involved in the control through incongruent dissolution reactions or surface processes whose net effect is to restrict the range of dissolved silica concentrations and the saturation state with respect to chalcedony as depth and residence times increase (Gimeno et al. 2009).

Eh values

Field potentiometrical measurements for the near-surface groundwaters in the Forsmark and Laxemar sites are not quality assured but the available data (e.g. Nilsson and Borgiel 2007, Gimeno et al. 2008, 2009) support the location of the oxic-anoxic transition already in these very shallow groundwaters (< 20 m depth). Moreover, dissolved redox-sensitive elements, indicating anoxic (post-oxic) and/or clearly reducing (sulphidic) conditions (e.g. Fe(II), S(-II)) show a wide variability and high contents in the near-surface groundwaters of both systems. Feasible redox potentials for the shallow groundwaters in post-oxic and sulphidic conditions may be inferred from the $Fe(OH)_3/Fe^{2+}$ (with the solubility value deduced by Banwart 1999) and from $S(-II)/SO_4^{2-}$ redox pairs, providing a range between −135 and −200 mV (Gimeno et al. 2008).

In situ redox potential measurements (with Chemmac) are available for deeper groundwaters in these sites. However, the number of Eh values obtained for the shallow groundwaters (< 200 m depth; Gimeno et al. 2008, 2009) is very low and, in most cases they correspond to brackish or saline groundwaters very different (chemical and hystorically, e.g. residence time) to what is expected for the fresh waters that will reach the SFR repository.

Nevertheless, some Eh values have been measured in dilute groundwaters in Laxemar barely affected by mixing. These dilute groundwaters (with chloride contents between 260 and 744 mg/L; Table 4-4) display considerably reducing values (–275 to –287 mV) for depths between 170 and 408 m.

Table 4-4. Available potentiometrically measured redox potentials (Eh) for fresh groundwaters in the Swedish sites.

Site	Borehole	Depth (m)	Cl (mg/L)	Eh (mv)	Source
Laxemar	KLX03	170.8	259.0	–275	Gimeno et al. 2009
	KLX13A	408.9	744.0	–287	
	KLX17A	342.3	565.0	–285	
	KLX17A	547.9	17.1	–303	
	KLX08	450.0	12.6	–266	
	KLX08	390.0	14.9	–245	
Fjällveden	KFI9	96.15	650.0	–250	Auqué et al. 2008
	KFI9	116.5	510.0	–250	

Some other waters, such as those in KLX17A and KLX08 boreholes, even more dilute (Cl between 14.9 and 17 mg/L; Table 4-4), with low drilling water percent and measurable tritium values, display even more reducing Eh values (from –245 to –303 mV). These values were measured at depths between 400 and 550 m in sections short-circuited during the measurement and, therefore, they would correspond to groundwaters from shallower levels (Gimeno et al. 2009). In any case, they would support the existence of very reducing conditions already in the recharge waters with very short residence time.

Finally, some Eh values (also obtained with Chemmac) are available for fresh groundwaters even at shallower levels (around 100 m depth; Table 4-4) in Fjällveden (Auqué et al. 2008), indicating, again, clearly reducing conditions (Eh = −250 mV).This fact would indicate the ability of microbial or water-rock interaction processes to create very reducing conditions at shallow depths.

With all these data, the Eh values proposed range from –135 to –300 mV.

Discussion and conclusions

Table 4-5 summarises the concentration ranges estimated for the fresh, near-surface and shallow groundwaters from the Forsmark and Laxemar sites and from Uppland and, in general, dissolved content and variation ranges are higher in the near surface than in the shallow groundwaters.

The highest values and broader ranges are found in the Forsmark site fresh near surface and fresh shallow groundwaters. This is especially important for alkalinity and calcium, reflecting the abundance of carbonates (calcite) in the Forsmark site overburden. Calcite presence in the overburden has been considered to predict the alkalinity in the largest lake expected to cover the area over one of the periods (the Lake Period, 4900 AD to 7500 AD in the SFR-1 Safety Analysis; SKB 2008a). Therefore, Forsmark site groundwaters waters in equilibrium with calcite seem to be the most suitable to define the ranges of carbonate system parameters.

As for the previous temperate case (repository covered by the sea), the proposed composition is given as a range, and a rounded value for all the parameters, is also indicated based on expert judgement. The proposed range (Table 4-5) has been mainly based on the values found in the fresh, shallow groundwaters from the Forsmark SDM dataset. If necessary, the usually wider values found in the near-surface groundwaters from the same Forsmark dataset can be used.

In general, composition and ranges suggested in this assessment are not very different from the values considered in the previous one (SFR 1; SKB 2008a). The ranges are slightly broader for elements such as sodium, potassium, calcium and magnesium. However, due to the available information at present, only groundwaters significantly unaffected by mixing have been used as representative of the ones derived from meteoric recharge, and therefore, the values for dissolved chloride are considerably lower (in the maximum and in the range: 500 mg/L vs 1,000 mg/L; Table 4-5). However, transition from the brackish or saline groundwaters present in the system, to the fresh waters towards the end of the period, will be gradual and, if necessary, broader ranges and/or higher values could be considered for dissolved chloride (e.g. 1,000 mg/L).

Table 4-5. Composition of penetrating fresh groundwater during a temperate climate domain when the repository is not covered by the sea[6]. For each parameter, proposed values are in bold and maximum and minimum values between brackets. Concentration ranges for the fresh near-surface (NSGW < 20 m depth) and fresh shallow groundwaters (FSGW 20 to 100 m depth) in the Forsmark and Laxemar sites, and in the Uppland area are also indicated. An alternative proposed composition for the climate case of "extended global warming" when a long temperate period is expected, is also indicated. Ion concentrations in mg/L. Data from the previous assessment (SKB 2008a) are shown for comparison.

	This Work **Proposed Composition**	**Ranges**						**Proposed Composition For A Long Temperate Period**	**Safetey Analyses SFR 1 (SKB 2008a)**
		Forsmark SDM		**Uppland**		**Laxemar SDM**			
		NSGW	**FSG**	**NSGW**	**FSG**	**NSGW**	**FSG**		
Tot number samples		**229**	**19**	**35**	**72**	**137**	**27**		
pH	**7.4 (6.6–8.3)**	6.6–7.9	7.07–7.81	–	–	6.35–8.57	–	7.6 (6.6–8.3)	**7.49** (6.7–8.7)
Eh	**–210 (–135 to –300)**	–	–135 to –200(2)	–	–	–	–240 to –300 (3)	–250 (–135 to –300)	**Red.** (–100, –400)
Cl	**190 (16–503)**	3.9–503	15.7–503	0.3–315	3.2–365	3.2–424	5.8–357	90 (5–357)	**45** (5, 1000)
SO_4^{2-}	**50 (25–163)**	0.75–251.1	25.3–163	7.2–84	7.9–187.7	0.81–176.2	17–110	40 (17–110)	**50** (3, 110)
HCO_3^- (Alk)	**300 (300–500)**	179–777	310–473	32–497	113–463	2.15–552	121–324	200 (120–324)	**300** (170, 540)
Na	**180 (65–400)**	4.6–500	64.6–399	1.8–255	3.4–285	4–249	38.4–248	110 (38–250)	**100** (20, 200)
K	**5 (5–15)**	1.56–37.6	5.6–15.3	0.9–42	1.2–51	0.97–46.3	1.8–5.35	3.0 (2–5.3)	**4** (0.2, 10)
Ca	**50 (24–105)**	29–232	23.9–102	22–142	9.6–197	2.7–104	7.5–48.3	30 (7–48)	**35** (25, 140)
Mg	**12 (7–24)**	4.15–63.2	6.9–23.4	1.4–13	0.97–14	0.88–45.2	1.9–12.9	6.0 (2–13)	**9** (3, 10)
SiO_2	**12 (2–21)**	2.16–29.9	13.3–20.9	–	–	9–72.5	12.6–31.2	10 (12–31)	**5.9**

[1] Data from Höglund(2001). These data are also presented in Table 6-12 from SKB (2008a).

[2] Deduced by means of redox pairs (see text).

[3] Potentiometrically measured Eh values in fresh groundwaters from Laxemar-Simpevarp and Fjällveden at depths between 100 to 550 m (Table 4-4).

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[6] This composition is also assumed for the periglacial climate domain when the repository is not covered by the sea (Section 4.2).

In the present assessment, proposed values for dissolved chloride and sodium are higher than in SFR1 (Table 4-5). These new concentrations are closer to the mean and median values for these elements in the fresh shallow groundwaters from the Forsmark site at present (see Table 4-3)[7]. In any case, the proposed range for chloride and sodium also include the selected values in the SFR1 assessment.

One of the biggest differences is in the dissolved silica. The contents proposed here are higher than those proposed in the previous SFR-1, where they were calculated assuming that the proposed groundwater was in equilibrium with quartz (Höglund 2001, SKB 2008a). Here the values have been selected from the values measured in the real waters where dissolved silica might not necessarily be controlled by a silica phase. Moreover, had these waters been in equilibrium with one of these phases, they would be with chalcedony or with the "new" quartz whose solubility data was proposed by Rimstidt (1997). Thus, some higher values, like those suggested in the present assessment, would be expectable.

As indicated above, the proposed composition for the fresh groundwaters (Table 4-5) represents a rounded composition with a percent error in the electrical balance of 0.55% and in equilibrium or near equilibrium with calcite (SI = – 0.09) and quartz[8] (SI = + 0.17, using the solubility data proposed by Rimstidt 1997). Overall, the proposed values for the different parameters (except those for Eh) are near the mean and median values presently found in the fresh shallow groundwaters from the Forsmark site (see Table 4-3).

Finally, an alternative reference water have been proposed for the climatic case of "*extended global warming"* based on the compositional characters of the fresh shallow groundwaters from the Laxemar site (Table 4-5). In this case, the percent error in the electrical balance is 1.5% and the water is also in equilibrium or near equilibrium with respect to calcite (SI = –0.24) and quartz (SI = + 0.09) at 15°C. Based on a review on the chemical compositions of groundwaters in crystalline systems not affected by mixing (recently perfomed by the authors of this report), the expected composition during this climate case would be closer to the lower limits of all the ranges proposed here.

4.2 Groundwater composition for the periglacial climate domain

This domain is defined as regions that contain permafrost. It is a cold region but without the presence of an ice sheet. The climate is colder than the temperate climate domain and warmer than the glacial climate domain. Precipitation may fall either as snow or rain. Within the periglacial climate domain, the site may also at times be submerged under the sea (see Chapter 3).

Depending on the climate case (Figure 3-1), this domain will start sooner or later in time and will last longer or shorter. For the *"global warming climate case"*, the first period of periglacial conditions will start after 50 ka of temperate climate domain, whilst for the *"extended global warming climate case"*, it will not start until after 100 ka of temperate conditions.

The two cases in which a periglacial domain can start earlier are "early periglacial climate case" and the "weichselian glacial cycle climate case". In the first one the initial period of temperate climate conditions is in this case only 15.5 ka long, followed by the first periglacial period (3 ka long). The climate is cold enough for shallow permafrost during this first periglacial period, but not cold enough for freezing of the concrete barriers of SFR. In the second, the periglacial domain will start even earlier and will alternate with warmer (temperate) periods for at least 55 ka until a glacial domain starts.

Under permafrost conditions, no great changes are expected in the salinity of the groundwaters when fresh or weakly brackish meteoric waters dominate the surface and the near-surface bedrock environment, that is, after a temperate period in which the repository is not covered by the sea. Salt exclusion due to freezing could increase the salinity of the groundwater (Vidstrand et al. 2007) but, if the groundwater is not particularly saline before the onset of permafrost, the effect of salt exclusion can probably be considered negligible (SKB 2010b).

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[7] TDS value for the proposed composition in the present assessment is 816.6 mg/L. For the SFR-1, this value is 562.3 mg/L.

[8] Saturation index calculations have been performed at 15°C.

There is very little information concerning the chemical characteristics of groundwaters related to permafrost conditions but it appears that most geochemical characteristics of groundwaters are almost unaffected by the permafrost. The available hydrochemical data at the Lupin Mine (Canada; Frape et al. 2004, Ruskeeniemi et al. 2004, Stotler et al. 2009) or at Greenland (Harper et al. 2011) indicate that the concentrations and pH values found in permafrost related groundwaters are mostly in the ranges proposed for the fresh groundwaters expected to be around the repository when it is not covered by the sea, during a temperate period (Table 4-5). Thus, the hypothetical reference groundwater expected to be around the repository during the *periglacial climate domain* would be similar to the groundwater proposed for the temperate domain when the repository is not covered by the sea (Table 4-5).

Brackish marine groundwaters are expected in the shallow bedrock under submerged conditions and the effects of salt exclusion may be more important during the development of permafrost in this case. The salts that are formed due to freezing are moved to the bottom of the permafrost and, thus, the deeper the permafrost, the greater salt exclusion could be. Since the repository is located at a shallow depth, the effect of salt exclusion may be limited. However, this aspect needs further studies. In any case, the proposal here is that the groundwater expected to be around the repository during the *periglacial climate domain* when the repository is coverd by the sea, could be similar to the brackish marine groundwaters selected for the temperate domain when the repository is also covered by the sea (Table 4-2).

4.3 Groundwater composition for the glacial climate domain

The glacial climate domain is defined as regions that are covered by glaciers or ice sheets which may, in some cases, be underlained by sub-glacial permafrost. The glacial climate domain has the coldest climate of the three climate domains (temperate, periglacial and glacial).These new climatic conditions will affect the composition of groundwaters reaching the repository. When the repository is located beneath a warm-based ice sheet, the inflowing meltwater will result in low salinity groundwater conditions.

Thus, considering the conditions expected for this climate domain, the reference groundwater that will reach the repository (in the case that it is located beneath a warm-based ice sheet) would have the composition of a dilute glacial meltwater (hereafter termed "glacial groundwater"). In the previous assessment (SFR 1; SKB 2008a) a chemical composition for this type of groundwater was not selected. In the present assessment, information and data available from the review performed by Gimeno et al. (2008, 2009) on the groundwaters of glacial origin identified during the SKB site investigations, and from the modeling calculations for the glacial end-member used in the SR-Can and SR-Site simulations (Auqué et al. 2006, Salas et al. 2010, Gimeno et al. 2010) have been used to propose a reference composition for this glacial groundwater.

4.3.1 Chemical composition of glacial derived groundwaters

The composition adopted for the glacial end member used for the modeling in the site investigation programmes (Table 4-6) corresponds to present melt-waters from one of the largest glaciers in Europe, the Josterdalsbreen in Norway, located on a crystalline granitic bedrock (Laaksoharju and Wallin 1997). The major element composition of these waters is similar to the one estimated by Pitkänen et al. (1999, 2004) for Olkiluoto (Finland). These glacial melt waters represent the chemical composition of surface melt waters prior to the water-rock interaction processes taking place during their infiltration into the bedrock. They have a very low content of dissolved solids, even lower than present day meteoric waters, a pH value of 5.8, and an isotopically light signature (Table 4-6).

The chemical composition of the Forsmark and Laxemar SDM groundwaters with glacial signatures has been drastically modified by mixing with waters of other origins (e.g. sample 1569 at Äspö, Table 4-6). Therefore, there are not "undisturbed" glacial melt water remnants that could be considered as a pure glacial component modified only by water-rock interaction processes. Nevertheless, the effect and extent of the expected water-rock interaction processes during the infiltration of glacial melt waters may be inferred from the study of waters in other zones not affected by mixing. The review performed by Gimeno et al. (2008, 2009) on the available data from the SKB Site Characterisation Programme different from the Laxemar and Forsmark sites (Ävrö, Bockholmen, Finnsjön, Fjällveden, Gideå, Kamlunge, Karlsham, Klipperås, Kråkemåla, Lansjärv and Svartboberget) has identified groundwaters of glacial or meteoric origin (but with high residence times) and corresponding to climates colder than at present (Table 4-7).

Table 4-6. Chemical composition of the glacial end-members used in the Swedish (Laaksoharju and Wallin 1997) and Finnish (Pitkänen et al. 1999, 2004) Site Characterisation Programmes. The composition of a present meteoric water with very low residence time together with one of the real samples with a clear glacial signature (Äspö groundwater, sample 1569), are shown. The Swedish glacial end member modified by water-rock interaction processes ("Equilibrated" glacial end member, as used in the SR-Can or SR-Site assessments; Auqué et al. 2006, Salas et al. 2010, Gimeno et al. 2010, and calculated in this work; see text) is also shown.

		Depth m	Temp °C	pH	Eh mV	Alkalinity mg/L	Cl	SO_4^{2-}	Ca	Mg	Na	K	SiO_2	Fe	δ^2H (‰)	$\delta^{18}O$
Glacial end member	Sweden			5.8	–	0.12	0.5	0.5	0.18	0.1	0.17	0.4	–		–158.0	–21.0
	Finland		1.0	5.8	–	0.16	0.7	0.05	0.13	0.1	0.15	0.15	0.011		–166.0	–22.0
"Equilibrated" Glacial end member (Sweden)	SR-Site		15	9.3		9.4	0.5	0.5	2.9	0.1	0.17	0.4	10.05		–	–
	This work		15	9.7		22.7	0.5	0.5	6.8	0.1	0.17	0.4	12.84		–	–
Meteoric water	HBH02 (#1931)		16	6.8	–	63.0	5.0	13.2	15.4	1.9	11.5	2.3	7.27		–77.1	–10.2
Äspö	KAS03 (#1569)	129–134	10.2	8.0	–280	61	1,220.0	31.1	162	21.0	613.0	2.4	10.48		–124.8	–15.8

Table 4-7. Compositional data for different groundwaters from a glacial infiltration or simply cold waters in different zones in Sweden and Switzerland. pH and Eh data in the Swedish sites have been obtained from the continuous logging with Chemmac (only pH data in bold and italics correspond to values determined in laboratory). Taken from Gimeno et al. (2008).

		Depth m	Temp °C	pH	Eh mV	Alkalinity mg/L	Cl	SO_4^{2-}	Ca	Mg	Na	K	SiO_2	Fe	δ^2H (‰)	$\delta^{18}O$
Fjallveden[1] Sweden	KFJ02 (#267)	605–607	–	8.9	–	83.0	170.0	0.2	12.0	0.8	130.0	1.0	9.1	0.34	–102.9	–14.11
	KFJ07 (#372)	542–544	–	**9.2**	–200	150.0	3.0	bdl.	10.0	2.0	46	3.6	n.a.	0.51	–	–
Gidea[2] Sweden	KGI04 (#194)	404–406	–	9.3	–200	18	178	0.1	21.0	1.1	105.0	1.9	10.0	0.07	–99.4	–13.63
Lansjärv Sweden	KLJ01 (#1410)	237–500	–	**9.2**	–	44.0	0.8	4.4	7.7	1.2	11.3	1.52	7.9	0.01	–109.6	–13.80
Svartboberget Sweden	KSV04 (#116)	430–436	–	9.1	–75	130.0	8.0	1.2	17.0	2.0	35.0	0.9	9.1	0.25	–95.0	–13.0
	KSV04 (#122)	630–633	–	9.1	–150	126.0	7.0	0.8	17.0	1.9	35.0	0.7	14.5	0.27	–95.4	–13.1
Switzerland	GTS[3]	450	12	9.6	–171	17.1	4.96	5.8	6.61	0.05	16.1	0.14	11.9	0.06	–	–

[1] Wallin (1995), Tullborg (1997), Bath (2005).

[2] Wallin (1995).

[3] Grimsel Test Site (Switzerland, Degueldre 1994).

The quality of the hydrochemical data from those sites have not been evaluated with the same detail as for the Laxemar and Forsmark SDM groundwaters and contamination with drilling water and/or other groundwaters may affect the quality of some of these data. However, some indications of ancient glacial melt water are apparent. For example, groundwaters below 500 m depth in Fjällveden seem to be residual melt waters or alternatively meteoric waters from a colder climate (Wallin 1995, Tullborg 1997). A glacial origin for these groundwaters is suggested in the work from Bath (2005) where “apparent” ^{14}C ages of around 12,000 to 14,000 years (i.e. late glacial) are reported. At Gideå, there seems to be an indication of mixing between meteoric and post glacial melt-waters (Wallin 1995). Finally, groundwaters in Lansjärv also show the isotopically light signature ($\delta^2H = -109.3‰$ and $\delta^{18}O = -13.8‰$) typical of glacial or old meteoric waters from colder climates.

Compared with the original composition of glacial melt waters (compare values in Table 4-6 and Table 4-7), all the Swedish waters have a more alkaline pH (≥ 9) and higher TDS values as a consequence of water-rock interaction. The differences are of orders of magnitude, especially for chloride, sodium and alkalinity. However, the final salt contents are still very low in absolute terms, even taking into account potential contamination. This means that, as expected, water-rock interaction modifies the overall compositional characteristics in a quite limited scale, but pH values are clearly increased. Similar conclusions have been obtained when analysing other cold meteoric and glacial waters in crystalline basements. For example, groundwaters from a recent meteoric origin at 450 m depth in the crystalline rocks of the Grimsel Test Site (Switzerland) are also alkaline, with pH = 9.6, and very diluted (Degueldre et al. 1996) similar to the ones observed in the Swedish groundwaters (Table 4-7).

In the SR-Can and SR-Site performance assessments (Auqué et al. 2006 Salas et al. 2010, Gimeno et al. 2010), the original composition of glacial melt-waters (Table 4-6) were equilibrated with respect to some minerals to obtain the possible compositional characteristics of these waters after water-rock interaction in the upper parts of the bedrock. Equilibrium with respect to quartz[9] and kaolinite were assumed and calcite saturation index was fixed to −1.0 (originally glacial meltwaters are strongly undersaturated with respect to calcite). The redox potentials were assumed to be controlled by an iron mineral phase (microcrystalline $Fe(OH)_3$) common in environments that buffer the input of oxygenated waters (see section on “Eh values”). The resulting groundwater composition (also displayed in Table 4-6) shows a TDS ≈ 20 mg/L (with respect to a TDS ≈ 3 mg/L in the non-equilibrated, original composition of glacial melt-waters) and the contents of the parameters affected by the imposed mineral equilibria (pH, alkalinity, dissolved calcium and silica), although still low, approach those measured in the “real” glacial-derived groundwaters (Table 4-7).

If the same equilibrium assemblage is used but imposing equilibrium with respect to calcite (calcite saturation index = 0.0), the obtained groundwater composition shows a TDS ≈ 33 mg/L and the values for the affected parameters are well inside the range defined by the measured ones (compare Table 4-6 and Table 4-7).

Overall, both reviewed groundwater data and modeled results on the chemical composition of the glacial-derived groundwaters would support a very dilute character, even lower than that for the present day meteoric waters. The “equilibrated” glacial end-member, used in the SR-Can or SR-Site exercises or modified in this work, could be maintained as reference composition for the glacial-derived groundwaters to be used in this SFR assessment (SR-PSU).

4.3.2 pH values

All the Swedish glacial derived groundwaters reviwed by Gimeno et al. (2008) have a more alkaline pH (pH ≥ 9; Table 4-7) than the original composition of glacial melt-waters (Table 4-6), as a consequence of water-rock interaction processes during their infiltration into the bedrock. The required time to reach these alkaline characters might not be so long as suggested by the residence time of the examined groundwaters (Table 4-7). The presence of geochemically reactive minerals like calcite, even at the trace amounts found in many crystalline systems[10], exert an important control

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[9] Using the solubility data proposed by Rimstidt (1997).

[10] Calcite dissolution will be a more effective pH-control reaction than aluminosilicate dissolution as it is much faster (at near neutral pH, the dissolution rate of calcite is approximately 7 orders of magnitude faster than the dissolution of plagioclase e.g. White et al. 1999a, b).

in the compositional evolution of glacial melt-waters (Brown 2002, Mitchell and Brown 2007). This control is dominant in environments out of contact with the atmospheric CO_2 and where other sources of acidity (e.g. pyrite dissolution) are limited (calcite is one of the most abundant minerals at all depths in the fracture fillings of the Forsmark and Laxemar sites whereas pyrite is much more scarce and evenly distributed; Drake et al. 2006), as it occurs during the infiltration of melt waters in the bedrock.

For example, if the original Swedish glacial end member, presented in Table 4-6, dissolves 2.2 mg/L of calcite it would reach a saturation index (S.I.) value of –2.0 (a highly undersaturated state) but the pH would be 9.0. If the amount of dissolved calcite is 4.6 mg/L, the S.I. would be of –1.0 (still clearly undersaturated) but the pH would reach a value of 9.6. The participation of other feasible minerals considered in this evolution (e.g. equilibrium with respect to kaolinite and microcrystalline iron oxyhidroxides; Auqué et al. 2006, Salas et al. 2010) does not change significantly the obtained results. For instance, the Swedish Glacial end member equilibrated with kaolinite, microcrystalline iron oxyhidroxide and with calcite at a S.I. value of –2.0 would reach a pH value of 8.8 (dissolving 3 mg/L of calcite); and if the calculation is performed considering a S.I. value for calcite of –1.0, the final pH value would be 9.3 (dissolving 6.7 mg/L of calcite). This last situation corresponds to the glacial end-member composition used in the simulations performed for SR-Can (Auqué et al. 2006) and Sr-Site (Salas et al. 2010, Gimeno et al. 2010). Finally, if calcite equilibrium is assumed, pH values could be 9.7.

Minor amounts of calcite dissolution (even far from equilibrium conditions) could promote clearly alkaline conditions and, thus, this situation can be reached soon during the infiltration of glacial waters in the bedrock. Studies performed at present on the subglacial waters at the ice-bedrock interface in the Haut Glacier d'Arolla in Switzerland (developed on crystalline rocks with disseminated calcite; Brown et al. 1996, Brown 2002, Tranter et al. 2002) indicate that despite the existence of an atmospheric CO_2 contribution to the acidity of these waters or the presence of reactive sulphides, the measured pH values range from 7 to 9.1. These values support the ability of the calcite interaction to promote the alkaline conditions in the glacial melt water quite soon during its infiltration.

Thus, based on the analytical data of glacial groundwater samples and on the geochemical modelling reasoning, a range of pH values between 9.0 and 9.6 can be proposed for the glacial melt waters infiltrated in the bedrock.

4.3.3 Eh values

As already mentioned, chemical composition of groundwaters with glacial signatures in the Forsmark and Laxemar sites have been drastically modified by mixing with waters of other origins and, thus, most of the available Eh measurements in both areas correspond to brackish or saline groundwaters very different to what is expected for the dilute glacial-derived groundwaters. However, there are some Eh values for dilute groundwaters, barely affected by mixing, in the Laxemar area. These dilute groundwaters (with chloride contents between 260 and 744 mg/L; Table 4-4), although not glacial-derived, display considerably reducing values (–275 to –287 mV) for depths between 170 and 408 m. Some additional Eh values are available from the review performed by Gimeno et al. (2008) on the identified groundwaters of glacial origin from other SKB site investigations (Fjällveden, Gideå, and Svartboberget; Table 4-7). As for Forsmark and Laxemar site research programmes, those Eh values were obtained from the continuous logging with Chemmac and mildly reducing values were measured (from −75 to −200 mV; Table 4-7).

All these data would indicate the ability of microbial or water-rock interaction processes to create very reducing conditions at shallow depths during present and past (glacial) infiltration of dilute waters. The modelling results obtained in SR-Can and SR-Site exercises would support these results.

As stated above, in the SR-Can and SR-Site performance assessments (Auqué et al. 2006, Salas et al. 2010, Gimeno et al. 2010), the redox potential was assumed to be controlled by an iron mineral phase (microcrystalline $Fe(OH)_3$) and the possibility of redox disequilibria was taken into account by performingthe redox calculations with a "coupled" and an "uncoupled"[11] thermodynamic database (see Auqué et al. 2006 for a detailed explanation).

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[11] The "uncoupled" database was modified to prevent the redox pairs SO_4^{2-}/HS^- and HCO_3^-/CH_4 participating in the homogeneous redox equilibrium during the predictive simulations. The procedure followed to implement this modification is explained in Auqué et al. (2006). With the original "coupled" database (AMPHOS TDB; Salas et al. 2010), the resulting Eh values correspond to homogeneous redox equilibrium among all redox pairs including Fe(III)/Fe(II), SO_4^{2-}/HS^- and HCO_3^-/CH_4 couples.

The calculated Eh values in the SR-Site exercise were clearly reducing (from −150 to −300 mV; column A, Table 4-8). Alternatively, if calcite equilibrium is considered (instead of fixing a saturation index of −1), more reducing values are obtained (column B, Table 4-8). And, finally, if a crystalline Fe(III)-oxyhydroxide is considered (with the solubility value proposed by Grenthe et al. 1992) even more reducing Eh values are predicted (column C, Table 4-8). Overall, the modeled Eh values for the glacial groundwater are similar or even more reducing than the measured ones in past (glacial-derived) or recent (meteoric) infiltrating dilute groundwaters. Therefore, the range defined by the measured values (from −75 to −280 mV) can be conservatively selected.

This range of Eh values would correspond to a glacial groundwater after reacting with the fracture minerals in the bedrock and, thus, without meaningful contents of dissolved oxygen. However, glacial recharge melt waters are likely to contain dissolved oxygen in larger quantities than rain water and, initially, they will show oxidising Eh values.

Based on theoretical estimations, the initial dissolved oxygen concentrations in glacial melt waters may reach a range of 29 to 45 mg/L (e.g. Ahonen and Vieno 1994, Glynn and Voss 1999, Guimerà et al. 1999, 2006, Sidborn et al. 2011 and references therein) and, therefore, they could be 3 to 5 times greater than in water equilibrated with the atmosphere (Glynn and Voss 1999, Sidborn et al. 2011). Calculated Eh values for glacial melt-waters with such a high oxygen content would range from +600 to + 900 mV. These values are in agreement with those obtained for the intruding ice melting waters in the oxygen intrusion models developed for different safety assessments(e.g. from +710 to +864 mV; Guimerà et al. 1999, 2006) and, thus, can be used for these climate cases.

However, it must be taken into account that photosynthetic and heterotrophic microbial populations thrive (at present) on the surface of most studied glaciers and ice sheets and, in some cases, the biological activity is so high that these environments become anaerobic. Furthermore, below many studied glaciers there are anaerobic processes ongoing (Sidborn et al. 2011 and references therein). These observations suggest that considering such high oxygen concentrations (and the corresponding high Eh values) in the glacial recharge melt waters is highly conservative.

Table 4-8. Calculated Eh and pH values for the glacial end member used in the SR-Can and SR-Site performance assessments when the water is equilibrated with respect to different mineral assemblages and using an uncoupled (first Eh value in the range) or a coupled (last Eh value in the range) thermodynamic database (AMPHOS TDB; Salas et al. 2010). Calculated pH values are not affected by using a coupled or an uncoupled database.

	A **Quartz + kaolinite + calcite *(SI = –1.0)* + *microcrystalline* Fe(OH)$_3$**	**B** **Quartz + kaolinite + calcite *(SI = 0.0)* + *microcrystalline* Fe(OH)$_3$**	**C** **Quartz + kaolinite + calcite *(SI = 0.0)* + *crystalline* Fe(OH)$_3$**
Eh	−150 to −300 mV	−172 to −348 mV	−325 to −370 mV
pH	9.30	9.68	9.68

4.3.4 Discussion and conclusions

Table 4-9 summarises the concentrations and ranges estimated for the glacial groundwater reaching the repository during a glacial climate domain. The proposed concentrations of dissolved elements mainly derive from the glacial end-member (used in the Swedish Site Characterisation Programmes) equilibrated with respect to quartz, kaolinite and calcite; the defined ranges are those mainly deduced from the glacial-derived groundwaters presented in Table 4-7. For pH and Eh values, the ranges have been obtained from measured and modeled results and the mean values have been included in the proposed composition.

Overall, the "rounded" proposed composition for the glacial groundwater (Table 4-9) shows a percent error in the electrical balance of –4.21% and it is in equilibrium or near equilibrium with respect to calcite (SI = −0.12) and quartz (SI = +0.11, using the solubility data proposed by Rimstidt (1997) at 15°C.

Table 4-9. Composition and concentration ranges for the glacial-derived groundwater expected for the 20,000 AD–100,000 AD period. Ion concentrations in mg/L.

	Proposed composition	Range
pH	9.3	9.0 – 9.6
Eh	+400 mV	+900 to −280 mV
Cl	0.5	0.5–178.0
SO_4^{2-}	0.5	0.1–5.8
HCO_3^- (Alk)	22.7	17.0–150.0
Na	0.17	0.17–130.0
K	0.4	0.14–3.6
Ca	6.8	6.6–21.0
Mg	0.1	0.05–2.0
SiO_2	12.8	7.9–14.5

The proposed composition and ranges for the glacial groundwater can be compared with the predicted compositions obtained in the simulations performed in the SR-Site Performance Assessment for the glacial stage. In the Forsmark area (Salas et al. 2010), a glacial period of 18,850 years was simulated in 10 time steps, reproducing the advance and the retreat of the ice front, for three hydrological stages: i) when the ice front is advancing to the repository area (2,900 years, approximately); ii) when the repository is entirely covered by a warm-based ice sheet i.e. an ice sheet with basal melting (15,000 years); and, finally, iii) when the ice sheet is retreating (1,200 years) and the area is covered by a 100 m deep melt water lake (Figure 4-12 and Figure 4-13).

Significant changes in groundwater composition were predicted, under a warm-based ice sheet (stage ii), as soon as the ice front advances over the repository area. The computed salinity (TDS, Figure 4-12) was not homogeneously distributed and the calculated TDS can reach values up to 20 g/L in locations affected by upconing of Deep Saline waters under an advancing and a retreating warm-based ice sheet. However, in the upper part of the modeled domain (less than 100 m depth, at the level of SFR repository), TDS values would be lower than 2 g/L and, usually, lower than 40 mg/L (similar to the value for the proposed glacial groundwater in this work) in most of the simulated time-steps.

The results indicate that glacial conditions may result on a general increase of pH values. When the ice sheet remains over the candidate repository volume, most of simulated groundwaters were characterised by pH values between 7.25 and 8.25, obtaining maximum values of around 9.5 (Salas et al. 2010). At shallower levels, higher pH values, between 9.0 and 9.7 were obtained in agreement with the pH range proposed for the glacial groundwater (Table 4-9).

With respect to the calculated Eh values, two geochemical assumptions, namely equilibrium with respect to amorphous Fe(II)-sulphide and Fe(III)-oxyhydroxide, were simulated in the SR-Site in order to estimate the evolution of the redox potential for the glacial stage in the area of Forsmark (Salas et al. 2010). The most oxidizing values were computed under the assumptions of Fe(III)-oxyhydroxides equilibrium and they are presented in Figure 4-13 for the candidate repository volume. In the first stages of the glacial cycle, the redox potential showed a wide variability and maximum values, higher than –50 mV, were predicted in the shallower levels (<100 m depth) of the candidate area. However, when the ice sheet covers the area of the candidate repository volume, most of the computed Eh values were around −290 mV, or even lower. These values were maintained for the rest of the remaining glacial stages and would be in agreement with the proposed Eh range for the glacial groundwaters if oxygen intrusion is excluded (Table 4-9).

Overall, the proposed composition and ranges for the glacial groundwaters provides consistent characters with those predicted for the Forsmark area in the SR-Site exercise.

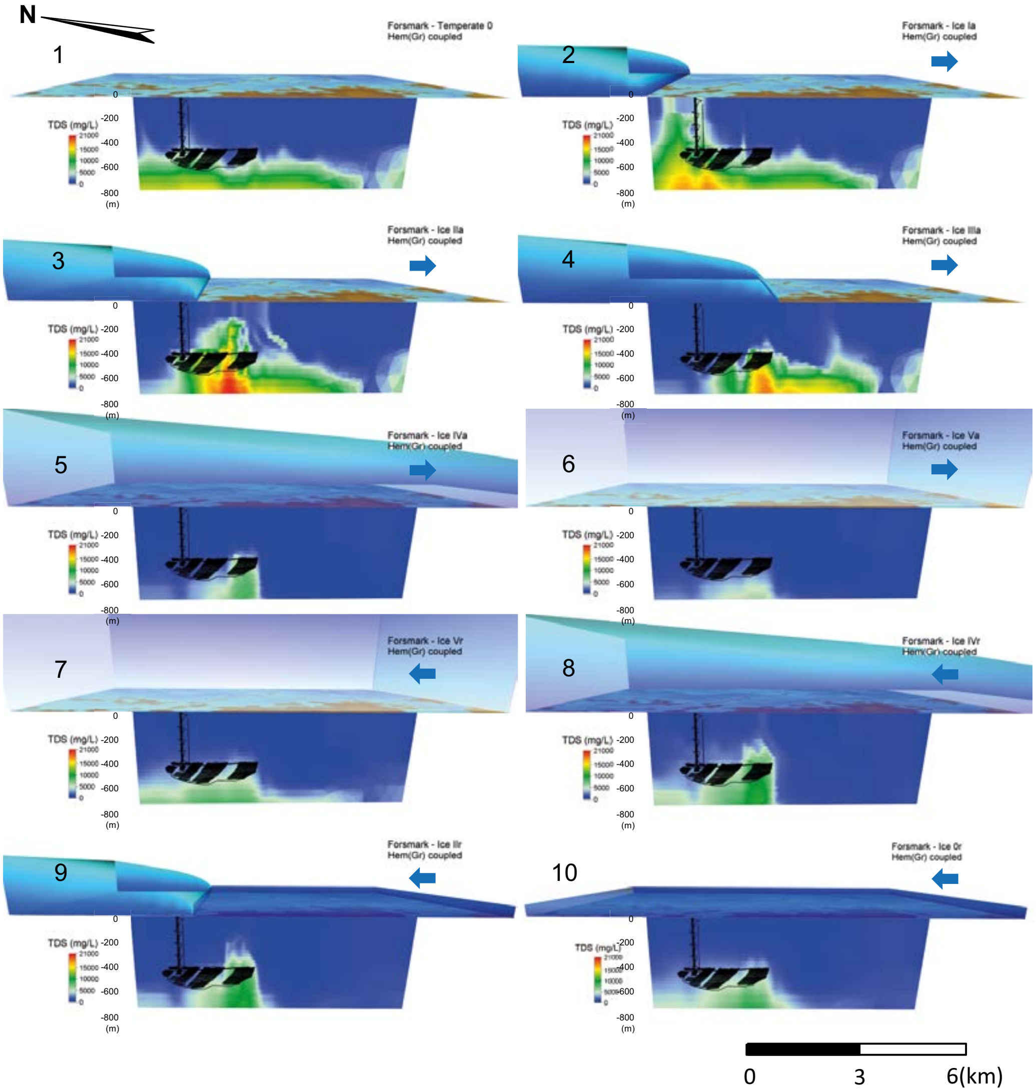

***Figure 4-12.** Changes in the distribution of TDS (total dissolved solids, mg/L) shown in vertical slices when an ice sheet advances and retreats over the unfrozen Forsmark area. The figure shows results during different stages on the glacial sheet advance (1 to 6) and the glacial retreat (7 to 10) over unfrozen ground. When the ice sheet retreats the area is covered by a 100 m deep glacial melt water lake. From Salas et al.(2010).*

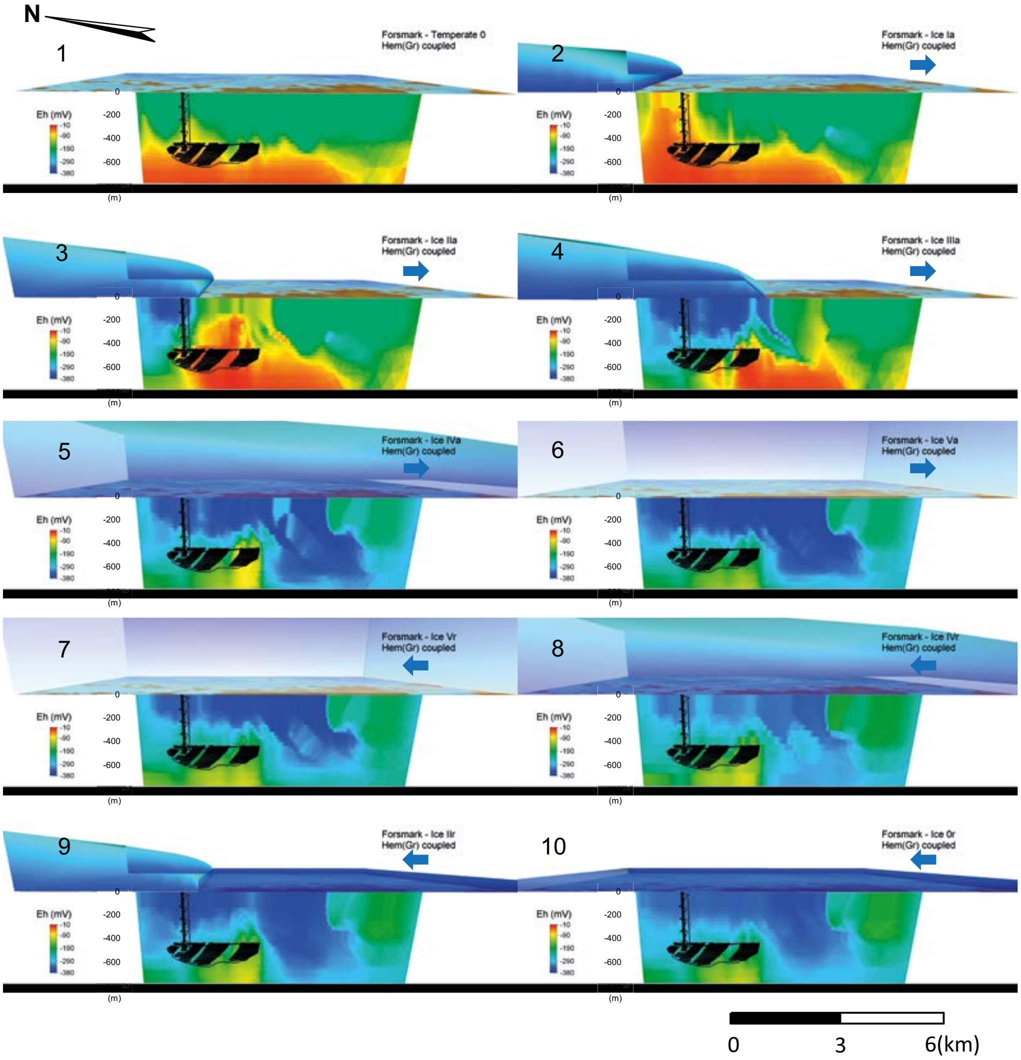

Figure 4-13. *Changes in the distribution of Eh, computed under the assumption of Fe(III) oxyhydroxides equilibrium, and shown in vertical slices when an ice sheet advances and retreats over the unfrozen Forsmark area. The figure shows results during the glacial sheet advance (1 to 6) and the glacial retreat (7 to 10) over unfrozen ground. When the ice sheet retreats the area is covered by a 100 m deep glacial melt water lake. From Salas et al.(2010).*

5 Conclusions

The aim of this study was to estimate reference chemical groundwater compositions (expected to be around the repository) under three different climate domains and submerged/emerged conditions in Forsmark to be used in the SR-PSU safety assessment.

The main bases for the selection of the proposed groundwater composition for these climatic domains are the chemical analyses, compilations, reviews and conclusions available from the site characterisation programmes of Forsmark, Laxemar and the SFR. Depending on the water type that is selected, different datasets were used and this is indicated in the Table headings.

The climate domains considered are: temperate, periglacial and glacial. Two possible situations will be considered for the *temperate domain*, the case of the site being submerged by the Baltic Sea (as today) and the case of the site above the sea level not covered by seawater due to the isostatic uplift. In the first case, an inflow of brackish-saline groundwater (similar to the situation at present) will dominate and the proposed composition is shown in Table 5-1. In the second case, land uplift will have proceeded so far that the groundwater flowing into the repository will be fresh (non-saline) having originated from recharge areas inland. The chemical composition for this groundwater is shown in Table 5-2.

There is very little information concerning the chemical characteristics of flowing groundwaters related to permafrost conditions although it appears that most geochemical characteristics of groundwaters are almost unaffected by the permafrost. With the available information, the groundwaters expected to be around the repository during the *periglacial climate domain* will be similar to the waters during the temperate domain when the repository is not covered by the sea (Table 5-2). Within this domain, the site may also at times be submerged under the sea and there are no data about the effects of freeze-out under this situation (see Section 4.2). The proposal here is that groundwaters could be similar to the brackish marine groundwaters proposed in Table 5-1 although this matter needs further studies.

Finally, for the *glacial domain* the repository will be located beneath an ice sheet and inflowing meltwater of low salinity will saturate the repository. The composition of this water is presented in Table 5-3.

Table 5-1. Composition of penetrating brackish saline groundwater and variation ranges for the parameters of interest for the temperate climate domain when the repository location is submerged under the sea. The proposed composition has been mainly based on the compiled groundwater dataset used for the SFR SDM (Nilsson et al. 2011, Gimeno et al. 2011) using only the available data for groundwaters down to –200 m depth.

	Composition	Range
pH	7.3	6.6–8.0
Eh (mV)	–225	–100 to –350
Cl (mg/L)	3,500	2,590–5,380
SO_4^{2-} (mg/L)	350	74–557.2
HCO_3^- (mg/L)	90	40–157
Na (mg/L)	1,500	850–1,920
K (mg/L)	20	3.8–60
Ca (mg/L)	600	87–1,220
Mg (mg/L)	150	79–290
SiO_2 (mg/L)	11	2.6–17.2

Table 5-2. Composition of the fresh groundwater around the repository during temperate and periglacial climate domains when the repository location is not covered by the sea. For the case with temperate and periglacial periods not extending for more than approximately 20–40 thousand years, the proposed composition has been based on the values found in the fresh, shallow groundwaters from the Forsmark SDM (< 100 m depth and Cl < 500 mg/L; Gimeno et al. 2008, Laaksoharju et al. 2008). An alternative proposed composition for the climatic case with temperate and periglacial periods with the repository location not covered by the sea extending for more than approximately 40 thousand years is also included, and are based on the fresh shallow groundwaters from the Laxemar SDM (Gimeno et al.2009).

	Temperate and periglacial periods not extending for more than approx. 20–40 ka.		Temperate and periglacial periods extending for more than approx. 40 ka	
	Composition	Range	Composition	Range
pH	7.4	6.6–8.3	7.6	6.6–8.3
Eh (mV)	−210	−135 to −300	−250	−135 to −300
Cl (mg/L)	190	16–503	90	5–357
SO_4^{2-} (mg/L)	50	25–163	40	17–110
HCO_3^- (mg/L)	300	300–500	200	120–324
Na (mg/L)	180	65–400	110	38–250
K (mg/L)	5	5–15	3.0	2–5.3
Ca (mg/L)	50	24–105	30	7–48
Mg (mg/L)	12	7–24	6.0	2–13
SiO_2 (mg/L)	12	2–21	10	12–31

Table 5-3. Composition and concentration ranges for the groundwater of glacial origin expected to reach the repository during a glacial climate domain. Concentrations of dissolved elements mainly derive from the modelling calculations performed for the glacial endmember used in the SR-Can and SR-Site simulations (Auqué et al. 2006, Salas et al. 2010, Gimeno et al. 2010) equilibrated with respect to quartz, kaolinite and calcite. For pH and Eh values, the ranges have been obtained from measured and modelled results.

	Composition	Range
pH	9.3	9.0 – 9.6
Eh (mV)	+400	+900 to −290
Cl (mg/L)	0.5	0.5–178.0
SO_4^{2-} (mg/L)	0.5	0.1–5.8
HCO_3^- (mg/L)	22.7	17.0–150.0
Na (mg/L)	0.17	0.17–130.0
K (mg/L)	0.4	0.14–3.6
Ca (mg/L)	6.8	6.6–21.0
Mg (mg/L)	0.1	0.05–2.0
SiO_2 (mg/L)	12.8	7.9–14.5

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Appendix A

Statistical calculations for different and supplementary datasets and sensitivity analysis

The selection of the reference waters for the temperate climate domain has been based on the chemical analysis available from different research programmes, mainly the Site Charaterisation Programmes in Forsmark, Laxemar and SFR (including groundwaters, GW, and near-surface groundwaters, NSGW). Additional data from wells, experiments, different controlling sampling campaigns and the ulterior monitoring programmes carried out in these sites have also been considered. Finally, a broad set of regional data from private wells in northern Uppland (defined by N: 6633169 - 6725589, E: 627152 - 733165, Sweref99TM) have been included in the analysis for comparison. The table delivered by SKB has been modified and the new file will be delivered associated with this report. The structure and content of this new file is explained in Appendix C.

As indicated in Chapter 4, the criteria has been to use those data already categorised in the previous hydrogeochemical works, considered as representative samples of the system. However, a comparison of the results obtained when using different datasets has been performed and it is included in this Appendix. The specific set of data used in each case (and the uncertainty analyses performed using different sets of data) is indicated in all the cases.

A1 Datasets used for the calculation of the water for the temperate climate domain with the repository submerged under the sea

The data used for the definition of this reference water (Table 4-2) include two different groups of samples from the SFR (see Section 4.1.1 for more details): (a) all the samples considered for the SDM (Nilsson et al. 2011) and (b) only the samples taken down to –200 m depth. Additionally, the Forsmark SDM groundwaters have also been considered as a comparative term and they have also been treated in another two groups: (c) all the samples taken down to 1,000 m depth, and (d) only the samples taken down to 200 m depth. For these two groups, only samples with categories 1 to 4 (considered representative of the system) have been included. The results were shown in Section 4.1.1 in Figure 4-10 and Table 4-1. The main differences among these different sets of datawere the following:

- Statistical differences between the values obtained with the two SFR sets (sets a and b, Table 4-1) are negligible and, as indicated in Section 4.1.1, and found only for the minimum values of some ranges Figure 4-10a and b).
- Statistical differences between the values obtained with the two Forsmark site subsets (sets c and d) are more significant and are associated with the different chemical compositions of the water types included in the two groups (Figure 4-10c and d). The most saline Forsmark groundwaters are not included in the second set (set d) as they are deeper than 200 m, and these waters show higher contents of Cl, Na or Ca and lower contents of HCO_3^- and Mg, for example.

Although not considered in Section 4.1.1, an additional test was made using not only the representative samples from Forsmark site dataset (categories 1 to 4) that correspond to sets c and d, but all the samples taken during the SDM studies, set c2 and d2 in Table A-1 and Figure A-1. The inclusion of these non-representative samples introduces important variations in some of the parameters with respect to what was found using only the representative ones:

- When using all the groundwaters at all depths (Figure A-1c), the maximum pH value is 9.69 (it was 8.4 with the representative ones, Figure A-1a) and the maximum silica and bicarbonate contents are also higher, 101.2 mg/L SiO_2 and 640 mg/L HCO_3^- (they were 33.8 mg/L and 473 mg/L, respectively); sodium, however shows a lower minium value, 28.8 mg/L while it was 64.6 mg/L (Figure A-1c).
- When using the groundwaters down to 200 m depth (Figure A-1d), the maximum for Ca is 1,980 mg/L (while it was 1,570 mg/L with the representative samples; Figure A-1b) and for HCO_3^- is 640 mg/L (473 mg/L); the minimum value for Na is 28.8 mg/L (64.6 mg/L).

Compared with the results obtained using the SFR data (Section 4.1.1) these variations are negligible: the main differences are due to the presence, in the Forsmark site, of meteoric waters in the first 200 m (not present at the SFR), and of more saline water below the –200 m depth.

Table A-1. Statistical values for only the *representative* waters (categories 1 to 4) taken at all depths in the Forsmark site (Set c), for *all* the waters (all categories) at all depths (set c2), for representative waters only down to 200 m (Set d) and for all the waters down to 200 m depth (Set d2).

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set c (Forsmark SDM groundwaters at all depths; only categories 1 to 4) (Figure A-1 a)										
pH	71	7.49	0.38	6.78	7.42	8.4	6.78	6.93	8.21	8.4
Eh	14	–211.00	43.63	–281	–201.5	–143	–281	–281	–143	–143
Na	139	1,452.75	656.55	64.6	1,570	3,130	64.6	229	2,290	3,130
K	139	23.53	15.05	4.88	20.8	67.8	4.88	6.02	58.7	67.8
Ca	139	1,111.44	1,255.03	23.9	860	6,520	23.9	33.7	3,980	6,520
Mg	139	105.33	80.54	3.87	106	287	3.87	7.57	242	287
HCO_3^-	139	165.04	136.70	5.72	126	473	5.72	8.42	450	473
Cl	139	4,278.76	3,041.14	15.7	4,120	15,000	15.7	145	10,500	15,000
SO_4^{2-}	139	292.05	171.44	25.32	320.56	587.19	25.32	47.63	560.23	587.19
SiO_2	139	13.96	3.87	2.61	13.99	33.80	2.61	8.64	20.92	33.80
Set c2 (Forsmark SDM groundwaters at all depths; all categories) (Figure A-1 b)										
pH	264	7.73	0.52	6.74	7.615	9.69	6.74	7.07	8.85	9.69
Eh	81	–206.74	45.09	–281	–196	–143	–281	–281	–143	–143
Na	743	1,473.86	660.62	28.8	1,590	3,130	28.8	205	2,270	3,130
K	743	20.09	12.66	4.51	16.7	69.4	4.51	6.02	45.5	69.4
Ca	743	1,347.72	1,302.72	23.6	1,070	6,560	23.6	37.5	4,140	6,560
Mg	743	89.76	82.08	2.57	52.5	289	2.57	7.66	235	289
HCO_3^-	739	143.53	142.85	3.42	101	640	3.42	7.84	450	640
Cl	743	4,763.02	3,166.33	9	4,830	15,000	9	139	10,500	15,000
SO_4^{2-}	743	249.52	168.95	16.84	189.94	614.16	16.84	49.13	548.25	614.16
SiO_2	743	14.82	6.83	1.45	14.10	101.19	1.45	8.64	23.53	101.19
Set d (Forsmark SDM groundwaters down to 200 m depth; only categories 1 to 4) (Figure A-1 c)										
pH	29	7.37	0.26	6.87	7.4	7.81	6.87	6.95	7.75	7.81
Eh	2	–191.50	4.95	–195	–191.5	–188	–195	–195	–188	–188
Na	69	1,094.81	659.70	64.6	1,240	2,210	64.6	156	2,000	2,210
K	69	28.36	17.65	4.88	26	67.8	4.88	5.64	60	67.8
Ca	69	423.37	410.83	23.9	311	1,570	23.9	30.2	1,220	1,570
Mg	69	111.19	82.61	6.91	132	287	6.91	7.57	246	287
HCO_3^-	69	257.25	132.53	61.5	236	473	61.5	98.8	461	473
Cl	69	2,474.31	1,891.49	15.7	2,630	5,980	15.7	60.8	5,421.7	5,980
SO_4^{2-}	69	297.51	164.80	25.3	338.5	587.2	25.3	47.6	548.2	587.2
SiO_2	69	14.25	3.46	2.6	14.4	21.4	2.6	10.1	19.1	21.4
Set d2 (Forsmark SDM groundwaters down to 200 m depth; all categories) (Figure A-1 d)										
pH	58	7.44	0.23	6.87	7.41	7.98	6.87	7.02	7.75	7.98
Eh	16	–191.06	3.59	–195	–188	–188	–195	–195	–188	–188
Na	309	1,032.40	682.59	28.8	1,110	2,240	28.8	148	2,000	2,240
K	309	478.21	428.73	23.6	400	1,980	23.6	29.7	1,260	1,980
Ca	309	23.66	15.48	4.51	21.5	69.4	4.51	5.6	56	69.4
Mg	309	102.07	82.69	5.83	102	289	5.83	7.43	240	289
HCO_3^-	305	267.29	140.22	61.5	239	640	61.5	96	480	640
Cl	309	2,478.06	2,004.40	9	2,590	6,030	9	58.9	5,410	6,030
SO_4^{2-}	309	274.06	166.55	16.84	282.81	614.16	16.84	47.63	536.26	614.16
SiO_2	309	14.90	2.95	2.61	14.63	23.53	2.61	10.63	20.82	23.53

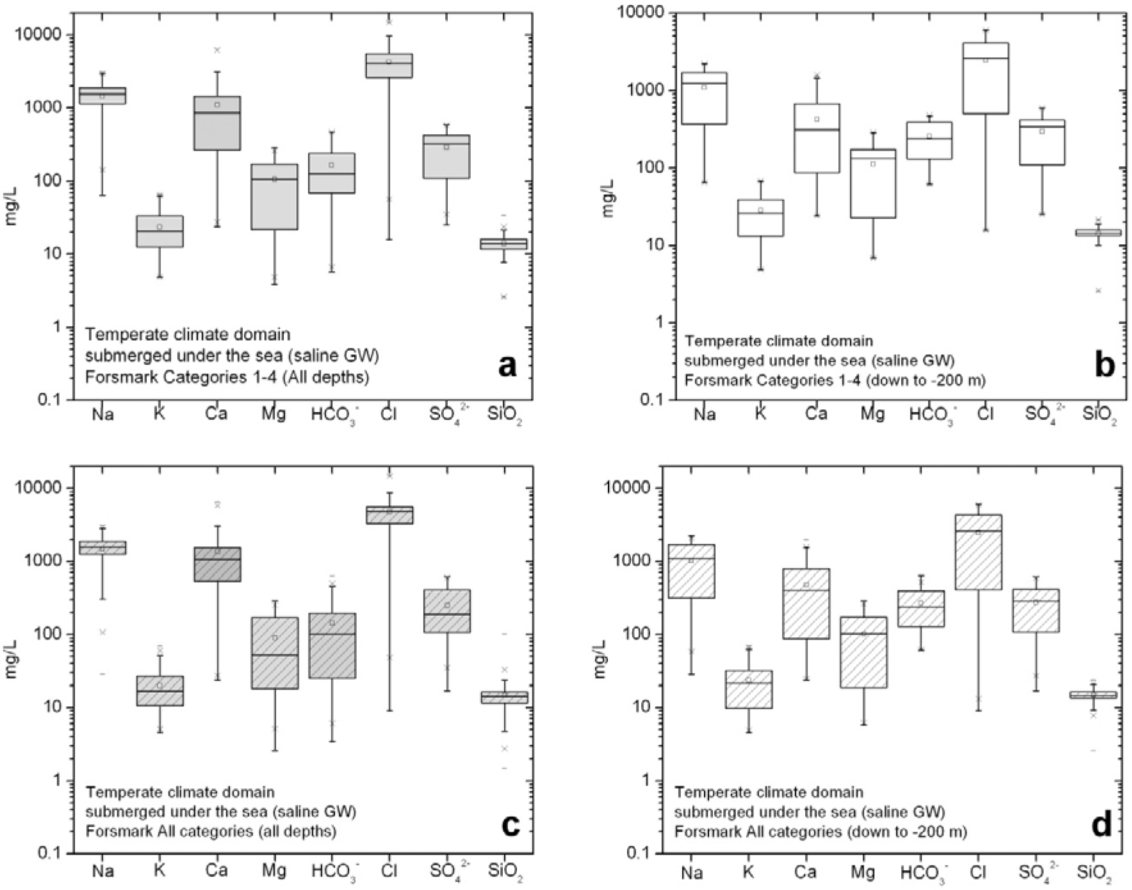

Figure A-1. *Box-and-whisker plots showing the comparison of the results obtained for the statistical distribution of the measured total concentration for the different major water components (in mg/L) in Forsmark SDM for the representative samples at all depths (a), for the representative samples located in the first 200 m depth (b), and for whole set of samples (all categories) at all depths (c) and only down to 200 m (d). The statistical measures plotted here and in all the following box and whiskers plots, are the median (horizontal line inside the grey box), the 25th and 75th percentiles (bottom and top of the box), the mean (square), the 5th and 95th percentiles ("whiskers"), the 1st and 99th percentile (crosses) and the maximum and the minimum values (horizontal bars).*

A2 Datasets used for the calculation of the reference water for the temperate climate domain with the repository not submerged under the sea

As explained in Section 4.1.2, due to the fact that there are not fresh meteoric groundwaters at the SFR, this reference water has been selected based on two groups of data: the fresh near surface (set 1) and the fresh shallow groundwaters (set 2) from the Forsmark site. Additionally, the same two groups of waters from the Laxemar site have been considered (sets 3 and 4) as an extreme case of more dilution if the temperate period above the sea is longer. Finally, the data from the Uppland area (separated in the two same sets) were taken into account for comparison in Section 4.1.2.

In this case, the influence of different cases is tested: a) the inclusion of other fresh water samples from the same sites (wells in Forsmark SDM and Uppland, and the samples taken in Ditches, Ponds, Surface and Wells in Laxemar SDM) and b) the inclusion of non representative waters in the Forsmark and Laxemar SDM groups.

Fresh Forsmark NSGW

Panels a and c in Figure A-2, show the different statistical results obtained for the representative near-surface groundwaters from the Forsmark site dataset (a) and for the group of waters including (together with these representative samples) the near-surface groundwaters from Uppland and some other near surface samples taken in wells in the Forsmark SDM area (c). The statistical distribution shown by the boxes (percentils 25 to 75) does barely change, and the same happens with the mean and median values, however, the extreme values (maximum and minimun) change clearly (Figure A-2a, c). For instance, the minimum for Mg changes from 4.15 to 0.11 mg/L, for Cl from 3.9 to 0.32 mg/L and, especially, for HCO_3^- from 179 to 32 mg/L. The maximum values for HCO_3^- and sulphate will increase quite more (from 777 to 840 and from 251 to 277 mg/L, respectively; Table A-2).

Figure A-2b and d show the results obtained when including the non-representative samples in the previous groups represented in panels a and b. Their inclusion modifies the ranges of some parameters (Table A-2). There is an increase in the maximum values for K (from 37.6 to 50.3 mg/L), HCO_3^- (from 777 to 870 mg/L), SO_4 (from 251.1 to 458 mg/L), SiO_2 (from 29.9 to 47.07) and Mg (from 63.2 to 95.8 mg/L) and a decrease in the minimum value for Ca (from 29 to 13.2 mg/L). That is, the inclusion of the non-representative samples introduces important changes.

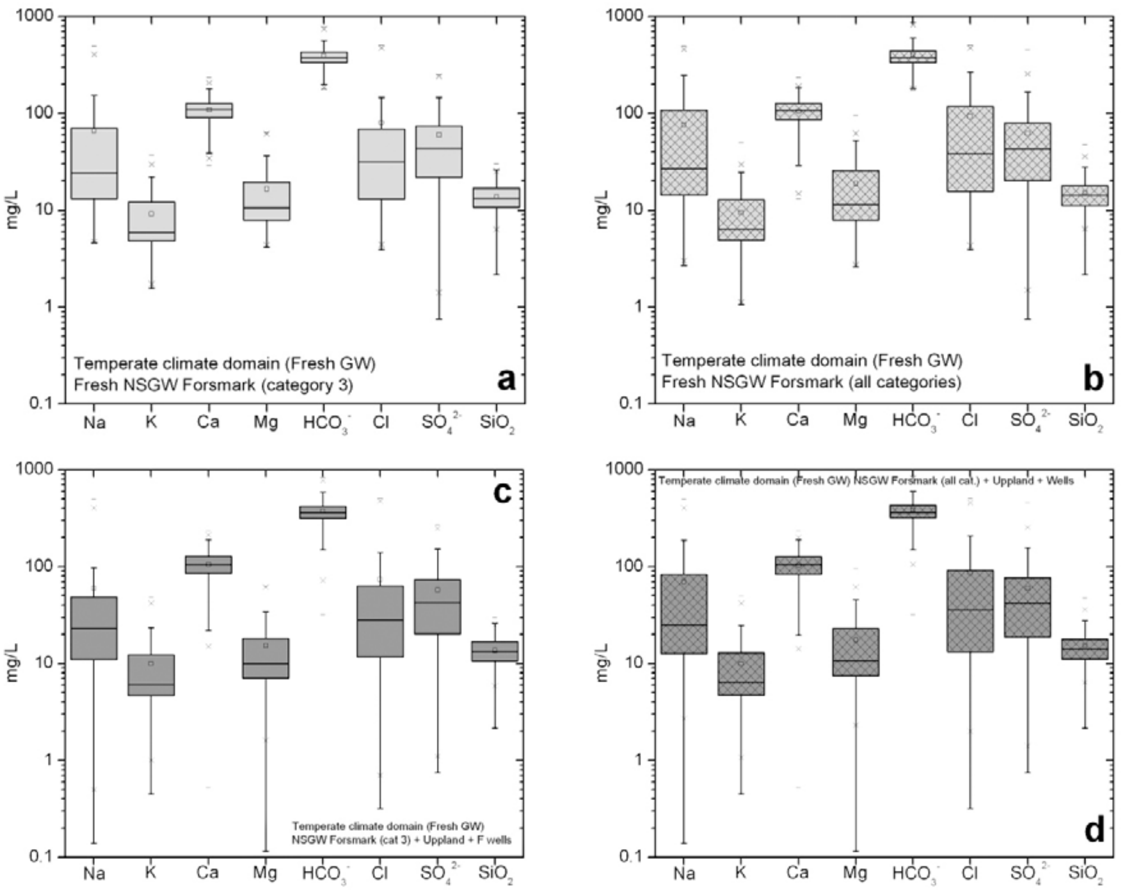

Figure A-2. Box-and-whisker plots showing the comparison of the results obtained for the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the fresh near-surface groundwaters from Forsmark SDM, only category 3 (a) and all the samples (b),and in all the available fresh near-surface groundwaters from Forsmark SDM (category 3 in panel c, and all categories in panel d) and from the wells in Uppland and Forsmark SDM areas. See the caption of Figure A-1 for the statistical meaning of the different symbols.

Table A-2. Statistical values for the fresh waters (Cl < 500 mg/L) taken near the surface (down to –20 m depth at the most; NSGW) in the Forsmark site considering only category 3 samples (set a), considering all the samples (set b), and including the rest of the near-surface groundwaters taken from wells in the Forsmark site and in the Uppland area together (sets c and d).

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set a, Fresh NSGW from Forsmark SDM (only category 3) (Figure A-2 a)										
pH	147	7.09	0.24	6.6	7.07	7.9	6.6	6.73	7.55	7.9
Na	229	66.37	95.01	4.6	24.3	500	4.6	5.8	283	500
K	229	9.16	7.24	1.56	5.92	37.6	1.56	2.23	26.5	37.6
Ca	229	108.25	35.22	29	110	232	29	39.7	169	232
Mg	229	16.59	13.79	4.15	10.6	63.2	4.15	4.88	50.4	63.2
HCO_3^-	229	392.49	111.61	179	374	777	179	229	615	777
Cl	229	80.24	114.82	3.9	31.5	503.3	3.9	6.6	370	503.3
SO_4^{2-}	228	60.04	53.36	0.7	43.6	251.1	0.7	3.2	178.0	251.1
SiO_2	229	13.74	4.29	2.2	13.3	30.0	2.2	7.3	20.7	30.0
Set b, Fresh NSGW from Forsmark SDM (all categories) (Figure A-2 b)										
pH	153	7.10	0.24	6.6	7.08	7.9	6.6	6.72	7.61	7.9
Na	350	75.53	98.83	2.7	26.75	500	2.7	5.9	287	500
K	350	9.43	7.22	1.06	6.49	50.3	1.06	2.08	24.6	50.3
Ca	351	105.09	35.07	13.2	108	232	13.2	39.7	158	232
Mg	351	18.75	15.84	2.6	11.4	95.8	2.6	4.67	57.2	95.8
HCO_3^-	344	401.67	129.07	173	374	870	173	213	688	870
Cl	351	93.45	121.07	3.9	38.1	506	3.9	5.3	371	506
SO_4^{2-}	351	62.00	63.96	0.75	42.84	458.37	0.75	3.03	187.84	458.37
SiO_2	351	15.35	6.15	2.16	14.21	47.07	2.16	7.49	29.95	47.07
Set c, Fresh NSGW from: Forsmark SDM (only category 3) + Uppland + Wells (drilled and excavated) (Figure A-2 c)										
pH	147	7.09	0.24	6.6	7.07	7.9	6.6	6.73	7.55	7.9
Na	293	60.04	89.39	0.14	23	500	0.14	5.1	266	500
K	291	9.94	9.34	0.45	6.05	48	0.45	1.94	29.6	48
Ca	290	106.02	39.75	0.53	106	232	0.53	35.9	180	232
Mg	293	15.32	13.10	0.115	10	63.2	0.115	4.16	45.7	63.2
HCO_3^-	292	375.91	134.00	32	362.5	840	32	181	665	840
Cl	294	73.91	110.12	0.32	28.6	503.3	0.32	4.4	354	503.3
SO_4^{2-}	294	57.15	52.62	0.7	42.5	270.0	0.7	3.2	157.0	270.0
SiO_2	230	13.68	4.37	0.1	13.3	30.0	0.1	7.3	20.7	30.0
Set d,Fresh NSGW from: Forsmark SDM ((all categories)+ Uppland + Wells (drilled and excavated) (Figure A-2 d)										
pH	153	7.10	0.24	6.6	7.08	7.9	6.6	6.72	7.61	7.9
Na	414	69.64	94.92	0.14	25.25	500	0.14	5.1	274	500
K	412	9.94	8.75	0.45	6.42	50.3	0.45	1.94	28.4	50.3
Ca	412	103.99	38.27	0.53	106	232	0.53	35.9	170	232
Mg	415	17.51	15.25	0.115	10.7	95.8	0.115	4.16	55.7	95.8
HCO_3^-	407	388.35	142.13	32	365	870	32	185	709	870
Cl	416	86.91	117.53	0.32	35.75	506	0.32	4.6	370	506
SO_4^{2-}	417	59.65	62.03	0.75	42.24	458.37	0.75	3.03	186.04	458.37
SiO_2	352	15.31	6.20	0.06	14.18	47.07	0.06	7.44	29.95	47.07

Fresh Laxemar NSGW

As for the NSGW from Forsmark SDM, apart from the category 3 NSGW samples from Laxemar SDM (Figure A-3a), here other sets of near-surface groundwaters taken from ditches, ponds, surface and wells in the Laxemar site have been considered (Figure A-3c). Compared with the results obtained for the fresh NSGW of category 3 (Table A-3), when including the additional sets of data, the statistical values (percentils 25 and 75, mean and median) do not change very much, although the extreme values do. The minimum value for SiO_2 changes from 9.1to 0.28 (Figure A-3a and c; Table A-3) and the maximum values for several elements also change, from 249 to 400 mg/L for Na, from 104 to 145 for Ca, from 45.2 to 52 for Mg, from 552 to 617 for alkalinity, from 424 to 500 for Cl, and from 176.2 to 200 mg/L for SO_4^{2-}.

The inclusion of non-representative samples in the two previous groups introduces additional modifications (Figure A-3b and d), mainly in Na (maximum of 420 mg/L), SO_4^{2-} (224.9 mg/L) and Cl (503 mg/L).

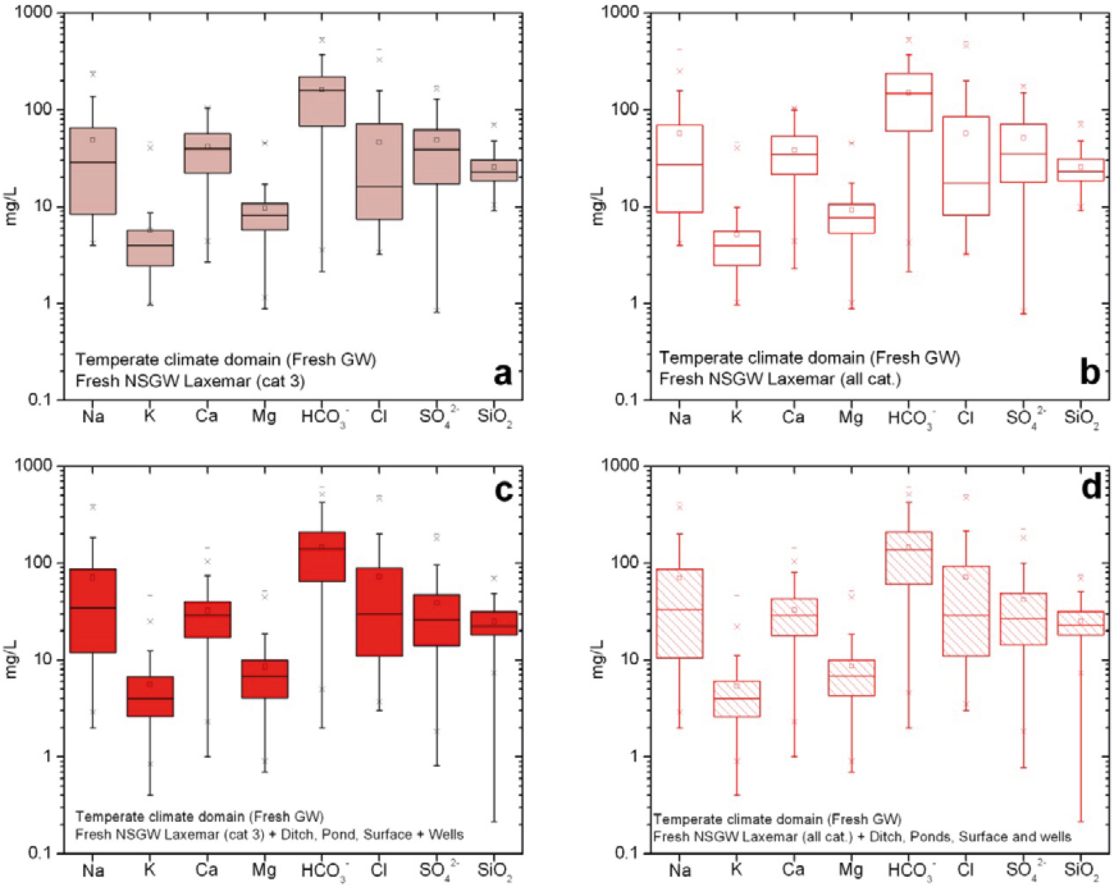

Figure A-3. *Box-and-whisker plots showing the comparison of the results obtained for the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the fresh near-surface groundwaters from Laxemar, only category 3 (a) and all the samples (b), and in the whole set of fresh near-surface groundwaters including wells, ditches and ponds (c, with category 3 samples, and d with all the samples). See the caption of Figure A-1 for the statistical meaning of the different symbols.*

Table A-3. Statistical values for the fresh waters (Cl < 500 mg/L) taken near the surface (down to –20 m depth at the most) in Laxemar considering only category 3 samples (set a), considering all the samples (set b), and including the rest of the near-surface groundwaters taken from wells, ditches and ponds in the same area of Laxemar (set c, with category 3 samples and d, with all the samples).

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set a, Fresh NSGW from: Laxemar SDM (category 3) (Figure A-3 a)										
pH	60	7.47	0.42	6.35	7.465	8.57	6.35	6.8	8.135	8.57
Na	137	48.87	58.86	4	28.8	249	4	4.9	213	249
K	137	5.74	7.23	0.97	4.01	46.3	0.97	1.13	13.5	46.3
Ca	137	41.75	22.99	2.7	39.7	104	2.7	9.1	81.3	104
Mg	137	9.66	8.29	0.88	8.1	45.2	0.88	2.29	28.8	45.2
HCO_3^-	137	160.73	110.76	2.15	160	552	2.15	20.2	301	552
Cl	137	46.14	62.19	3.2	16.1	424	3.2	4	147	424
SO_4^{2-}	137	48.86	39.24	0.8	38.9	176.2	0.8	7.8	139.6	176.2
SiO_2	137	25.58	10.60	9.1	22.7	72.5	9.1	13.6	44.3	72.5
Set b, Fresh NSGW from: Laxemar SDM (all categories) (Figure A-3 b)										
pH	70	7.45	0.43	6.27	7.465	8.57	6.27	6.8	8.11	8.57
Na	260	57.49	73.54	4	27.3	420	4	5.4	222	420
K	260	5.17	5.56	0.97	4	46.3	0.97	1.305	12.4	46.3
Ca	260	38.16	21.56	2.3	35.05	104	2.3	8.35	71.75	104
Mg	260	9.26	7.61	0.88	7.66	45.2	0.88	2.52	23.6	45.2
HCO_3^-	259	150.20	104.18	2.15	147	552	2.15	17.7	276	552
Cl	260	57.06	80.83	3.2	17.55	503	3.2	4	162.5	503
SO_4^{2-}	260	51.38	44.41	0.78	35.35	182.75	0.78	7.77	153.39	182.75
SiO_2	259	25.47	10.42	9.14	23.11	74.66	9.14	11.94	43.43	74.66
Set c, Fresh NSGW from: Laxemar SDM (Cl < 500)+ Ditch + Ponds and surf. + drilled and excav. (Figure A-3 c)										
pH	60	7.47	0.42	6.35	7.465	8.57	6.35	6.8	8.135	8.57
Na	536	71.30	89.94	2	34.3	400	2	4.6	280	400
K	520	5.60	5.27	0.4	4.01	46.3	0.4	1.12	14.5	46.3
Ca	536	32.27	22.19	1	29	145	1	5	74	145
Mg	532	8.53	7.43	0.7	6.83	52	0.7	1.2	23	52
HCO_3^-	506	147.64	100.27	2	140	617	2	11	310	617
Cl	528	72.14	97.77	3	30	500	3	5.7	320	500
SO_4^{2-}	531	38.87	38.12	0.8	26.0	200.0	0.8	7.5	120.0	200.0
SiO_2	171	25.09	11.03	0.28	22.2	72.5	0.2	11.7	44.3	72.5
Set d, Fresh NSGW from: Laxemar SDM (all cat.) + Ditch + Ponds and surf. + drilled and excav. (Figure A-3 d)										
pH	70	7.45	0.43	6.27	7.465	8.57	6.27	6.8	8.11	8.57
Na	661	70.46	89.13	2	33	420	2	4.6	260	420
K	645	5.39	4.88	0.4	4	46.3	0.4	1.22	13.2	46.3
Ca	661	32.70	21.83	1	29	145	1	5.2	72.6	145
Mg	657	8.61	7.37	0.7	6.86	52	0.7	1.34	23.3	52
HCO_3^-	630	145.40	99.48	2	138.5	617	2	10.8	292	617
Cl	653	71.78	97.61	3	29	503	3	5.1	320	503
SO_4^{2-}	656	41.99	41.48	0.78	27.00	224.99	0.78	7.55	148.30	224.99
SiO_2	295	25.10	10.74	0.21	22.68	74.66	0.21	11.62	44.07	74.66

Fresh Shallow groundwaters from Forsmark SDM

As indicated in Section 4.1.2, the most suitable set of samples to select the hypothetical reference water for this temperate climate domain when the repository is not submerged under the sea, would be the fresh shallow groundwaters from the Forsmark site. This set, with only the samples from categories 1 to 4, and the fresh shallow groundwaters from the whole area of Uppland were shown in Section 4.1.2. Here, three additional sets of samples are tested. The first one (set b in Table A-4) includes all the fresh shallow samples from Forsmark SDM (all categories), the second one (set c in Table A-4), includes the samples from set a from Forsmark SDM and the samples from Uppland together. And the third one includes all the fresh shallow samples from Forsmark SDM (all categories) and the samples from Uppland together (set d in Table A-4).

Table A-4. Statistical values for the fresh shallow groundwaters (Cl < 500 mg/L) sampled down to –100 m depth at the most, in Forsmark SDM dataset considering only categories 1 to 4 (set a), considering all the samples (set b), the waters from Uppland (set c) and both sets together, set d only with the representative samples from Forsmark SDM and set e with all the fresh shallow groundwaters.

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set a: Fresh Shallow GW Forsmark SDM (categories 1 to 4) (Figure A-4 a)										
pH	9	7.51	0.27	7.07	7.58	7.81	7.07	7.07	7.81	7.81
Na	19	251.82	89.69	64.6	256	399	64.6	64.6	399	399
K	19	9.63	3.46	5.6	9.32	15.3	5.6	5.6	15.3	15.3
Ca	19	49.72	23.24	23.9	41.1	102	23.9	23.9	102	102
Mg	19	12.80	6.03	6.91	9.01	23.4	6.91	6.91	23.4	23.4
HCO_3^-	19	420.89	43.65	310	446	473	310	310	473	473
Cl	19	218.12	154.46	15.7	184	503	15.7	15.7	503	503
SO_4^{2-}	19	86.73	33.61	25.3	94.7	163.0	25.3	25.3	163.0	163.0
SiO_2	19	15.63	2.16	13.3	14.6	20.9	13.3	13.3	20.9	20.9
Set b: Fresh Shallow GW Forsmark SDM (all categories) (Figure A-4 b)										
pH	10	7.53	0.26	7.07	7.6	7.81	7.07	7.07	7.81	7.81
Na	78	229.77	94.84	28.8	242	545	28.8	64.6	398	545
K	78	8.52	3.09	4.51	7.695	17.6	4.51	5.26	14.3	17.6
Ca	78	58.30	36.88	23.6	41.8	167	23.6	25.2	158	167
Mg	78	11.91	5.68	5.83	9.44	34.9	5.83	6.11	22.8	34.9
HCO_3^-	77	432.47	55.96	231	446	640	231	360	513	640
Cl	78	188.27	133.33	12.6	163	503	12.6	14.3	467	503
SO_4^{2-}	78	83.06	33.63	24.15	83.73	164.17	24.15	27.26	152.19	164.17
SiO_2	78	15.64	2.38	9.22	15.80	21.22	9.22	11.89	19.40	21.22
Set c: Fresh Shallow GW from Forsmark SDM (categories 1 to 4) and Uppland (Figure A-4 c)										
pH	9	7.51	0.27	7.07	7.58	7.81	7.07	7.07	7.81	7.81
Na	91	106.94	99.32	3.4	75	399	3.4	4.8	339	399
K	91	8.37	9.03	1.2	5.64	51	1.2	1.6	27	51
Ca	86	61.93	37.41	9.6	54.1	197	9.6	15	133	197
Mg	91	7.58	4.64	0.97	7.2	23.4	0.97	2.2	19.7	23.4
HCO_3^-	90	311.38	87.59	113	309.5	473	113	175	461	473
Cl	91	86.59	115.84	3.2	31	503	3.2	6.1	365	503
SO_4^{2-}	91	45.41	40.24	7.9	31.0	187.7	7.9	10.0	110.8	187.7
SiO_2	19	15.63	2.16	13.3	14.6	20.9	13.3	13.3	20.9	20.9
Set d: Fresh Shallow GW from Forsmark SDM (all categories) and Uppland (Figure A-4 d)										
pH	10	7.53	0.26	7.07	7.6	7.81	7.07	7.07	7.81	7.81
Na	150	152.46	113.01	3.4	143.5	545	3.4	7.4	343	545
K	150	8.29	7.25	1.2	6.595	51	1.2	2.3	21	51
Ca	145	61.58	38.38	9.6	52	197	9.6	19	154	197
Mg	150	9.17	5.39	0.97	7.795	34.9	0.97	2.8	20.4	34.9
HCO_3^-	148	360.32	98.74	113	373	640	113	194	490	640
Cl	150	122.81	127.65	3.2	72.55	503	3.2	7.8	409	503
SO_4^{2-}	150	59.76	41.75	7.89	47.78	187.74	7.89	10.98	151.59	187.74
SiO_2	78	15.64	2.38	9.22	15.80	21.22	9.22	11.89	19.40	21.22

When the samples from all categories are included in any of the sets (only Forsmark SDM or Forsmark SDM and Uppland), the ranges of several elements increase (Na, Ca, Mg, HCO_3^-) and the minimum value for silica decreases (Table A-4).

The inclusion of the Uppland samples together with the Forsmark SDM dataset changes all the percentiles in the boxes and the contents of Na, K, Mg, HCO_3^-, Cl and SO_4^{2-} decrease considerably (Figure A-4). This change in the statistical distribution also affects the maximum and minimum values of almost all parameters. There is a decrease in the minimum of Na (from 64.6 to 3.4 mg/L), K (from 5.6 to 1.2), Ca (from 23.9 to 9.6), Mg (from 6.9 to 0.97), HCO_3^- (from 310 to 113), Cl (from 15.7 to 3.2) and SO_4^{2-} (from 25.3 to 7.9). And a paralell increase in the maximum of K (from 15.3 to 51), Ca (from 102 to 197) and SO_4^{2-} (from 163 to 187.7).

So, the inclusion of these additional sets would change almost all the ranges indicated in Table 4-5 for this reference water.

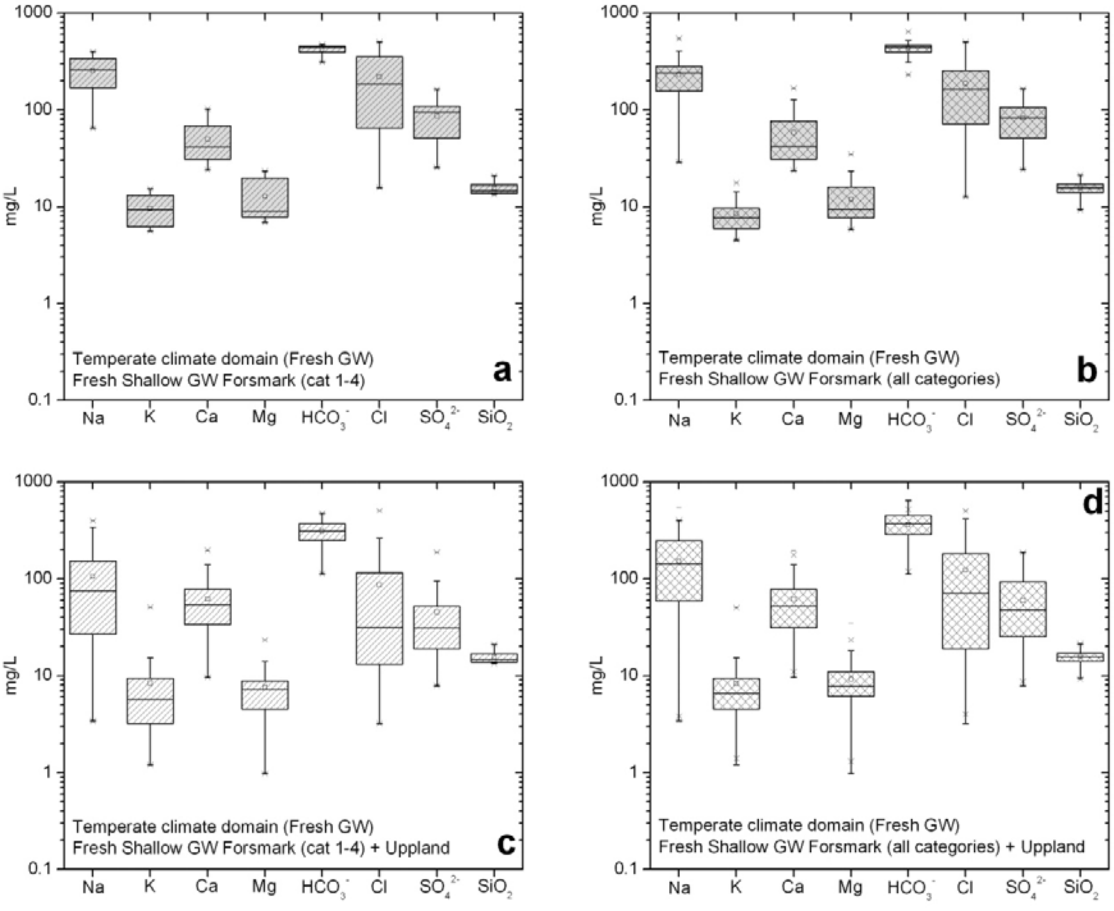

Figure A-4. *Box-and-whisker plots showing the comparison of the results obtained for the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the fresh shallow groundwaters from Forsmark SDM, only categories 1 to 4 (a) and all the samples (b), and in the whole set of fresh shallow groundwaters including Uppland samples (c, with categories 1 to 4 for Forsmark SDM samples, and d with all the samples). See the caption of Figure A-1 for the statistical meaning of the different symbols.*

Fresh Shallow groundwaters from Laxemar

In this case the comparison is easier as there is only an additional set of samples tested: the whole set of representative and non representative samples from the fresh shallow groundwaters from Laxemar.

With respect to the compositional ranges indicated in Table 4-5 (Section 4.1.2) based on the representative samples, the inclusion of the rest of the samples produces an increase in the maximum values for Na (from 248 to 430), Ca (from 48.3 to 54.5), Cl (from 357 to 440), SO_4^{2-} (from 110 to 260) and a decrease in the minimum values of HCO_3^- (from 121 to 51), SO_4^{2-} (from 17 to 6.11) and SiO_2 (from 12.6 to 3.2). The values are included in Table A-5 and the statistical plots in Figure A-5.

Table A-5. Statistical values for the fresh shallow groundwaters (Cl < 500 mg/L) sampled down to –100 m depth at the most, in Laxemar considering only categories 1 to 4 (set a) and considering all the samples (set b).

	Samples	Mean	Stand. Dev.	Min	Median	Max	P0.1	P5	P95	P99.9
Set a: Fresh Shallow GW Laxemar SDM (categories 1 to 4) (Figure A-5 a)										
pH	0	–	–	–	–	–	–	–	–	–
Na	27	120.49	53.02	38.4	110	248	38.4	41.7	217	248
K	27	3.33	0.96	1.77	3.17	5.35	1.77	2	5.32	5.35
Ca	27	22.47	12.61	7.5	17	48.3	7.5	9.6	46.4	48.3
Mg	27	4.60	2.35	1.9	4.09	12.9	1.9	2.23	8.32	12.9
HCO_3^-	27	230.04	44.05	121	224	324	121	157	311	324
Cl	27	68.88	77.60	5.8	43.6	357	5.8	8.2	203	357
SO_4^{2-}	27	47.83	23.06	17.0	49.1	109.6	17.0	20.8	99.2	109.6
SiO_2	24	15.66	3.77	12.6	14.8	31.2	12.6	12.8	20.7	31.2
Set b: Fresh Shallow GW Laxemar SDM (all categories) (Figure A-5 b)										
pH	5	8.19	0.23	7.93	8.17	8.56	7.93	7.93	8.56	8.56
Na	71	130.02	72.39	32.5	121	430	32.5	44.3	248	430
K	71	3.42	0.96	1.16	3.42	5.6	1.16	1.77	5.2	5.6
Ca	71	23.33	13.03	6.4	17.1	54.5	6.4	9.6	46.4	54.5
Mg	71	4.68	1.97	1.9	4.37	12.9	1.9	2.13	7.85	12.9
HCO_3^-	70	224.53	46.39	51	225	324	51	136	301	324
Cl	71	86.58	98.62	5.7	45.1	440	5.7	6.3	357	440
SO_4^{2-}	71	52.45	37.81	6.11	49.13	260.00	6.11	8.70	109.65	260.00
SiO_2	62	14.61	4.00	3.27	14.32	31.23	3.27	8.56	20.67	31.23

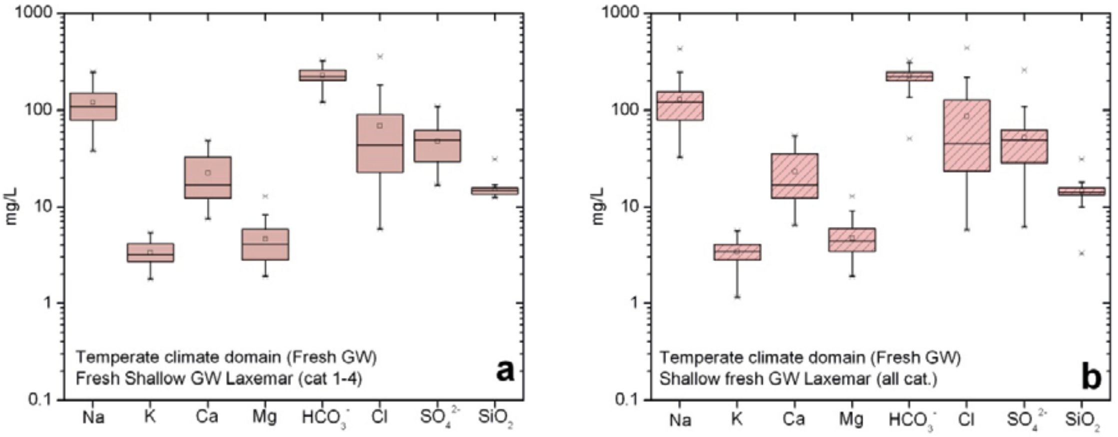

Figure A-5. *Box-and-whisker plots showing the comparison of the results obtained for the statistical distribution of the measured total concentration for the different major water components (in mg/L) in the fresh shallow groundwaters from Laxemar SDM, only categories 1 to 4 (a) and all the samples (b). See the caption of Figure A-1 for the statistical meaning of the different symbols.*

Appendix B

Dissolved organic carbon contents

The concentration of dissolved organic carbon (DOC[12]) is of special interest for microbiological interpretations as it can be used as a source of energy, electrons and carbon by heterotrophic microorganisms, and it is produced by autotrophic microorganisms (e.g. acetate). DOC contents may favour reducing conditions through microbial activities but may also have detrimental effects (e.g. the formation of organic complexing compounds and organic colloids might enhance the potential for radionuclide transport; Salas et al. 2010, Gimeno et al. 2010).

Thus, it is necessary to assess the possible contents of DOC for the groundwaters related with the different climate domains (temperate, periglacial and glacial domains) considered in this study.

The sources of data and criteria for this assessment are mainly the same as those used in the selection of the reference waters (Chapter 4), that is, data from the Site Charaterisation programmes in Forsmark, Laxemar and SFR (including groundwaters, GW, and near-surface groundwaters, NSGW). Regional data from private wells in northern Uppland have not been considered as they do not include data on TOC or DOC.

The criterion to select the data has been to use those already checked and considered as representative of the system in the previous hydrogeochemical works. There is very little information concerning the DOC contents and the chemical characteristics of groundwaters related to permafrost and glacial conditions and in those cases a review of the still scarce available information about this subject has been performed.

B1 DOC contents in the SFR groundwaters and other crystalline systems

DOC contents in the SFR groundwaters range from 0.7 to 5.1 mg/L (0.06 to 0.42 mmol/L; Figure B-1a and Table B-1) with a mean value of 1.85 mg/L (≈ 0.15 mmol/L). There is no specific trend versus depth but the highest variability and also the highest DOC contents have been measured in the upper 200 m (between 95 and 160 m depth; Figure B-1a) associated to Littorina and Glacial type groundwaters. However, it is only in these water types where DOC contents below the detection limit have been found (9% of the analysed Littorina-type groundwaters and 23% of the analysed Glacial-type).

The DOC analysed in the Baltic type groundwaters ranges from 1.7 to 3.0 mg/L (0.14 to 0.25 mmol/L; Table B-1) and the mean value is higher than in any of the other groundwater types. However, these waters show a narrower range and lower maximum value than the rest of the groundwater types and than the Baltic Sea waters near the SFR (between 1 and 6 mg/L; Figure B-1a) and they do not reach values higher than 3 mg/L, frequently observed in the marine waters (Figure B-1a).

These data indicate that the present intrusion of Baltic waters in the SFR has favoured a pervasive presence of meaningful amounts of DOC in the affected resident groundwaters. The fact that the values found in these groundwaters are not as high as the typical marine waters is probably related to the microbial activity, which decreases the DOC content during infiltration (see Gimeno et al. 2011 and references therein).

Dissolved organic contents were also measured in the Forsmark site at all depths, the near surface, the shallow and the deep groundwaters (Figure B-1b). DOC and TOC contents in the near-surface groundwaters (down to 10–20 m depth) range from 2 to 40 mg/L (0.17 to 3.33 mmol/L) although 75% of the samples show concentrations below 16.5 mg/L (1.37 mmol/L; Tröjbom and Söderbäck 2006a). Fresh and shallow (< 100 m) groundwaters show a narrower range and lower maximum DOC values, between 6 and 13 mg/L (0.5 to 1.08 mmol/L; Figure B-1b), which is also consistent with the decrease of DOC contents, due to microbial activity, during the infiltration of the present meteoric waters.

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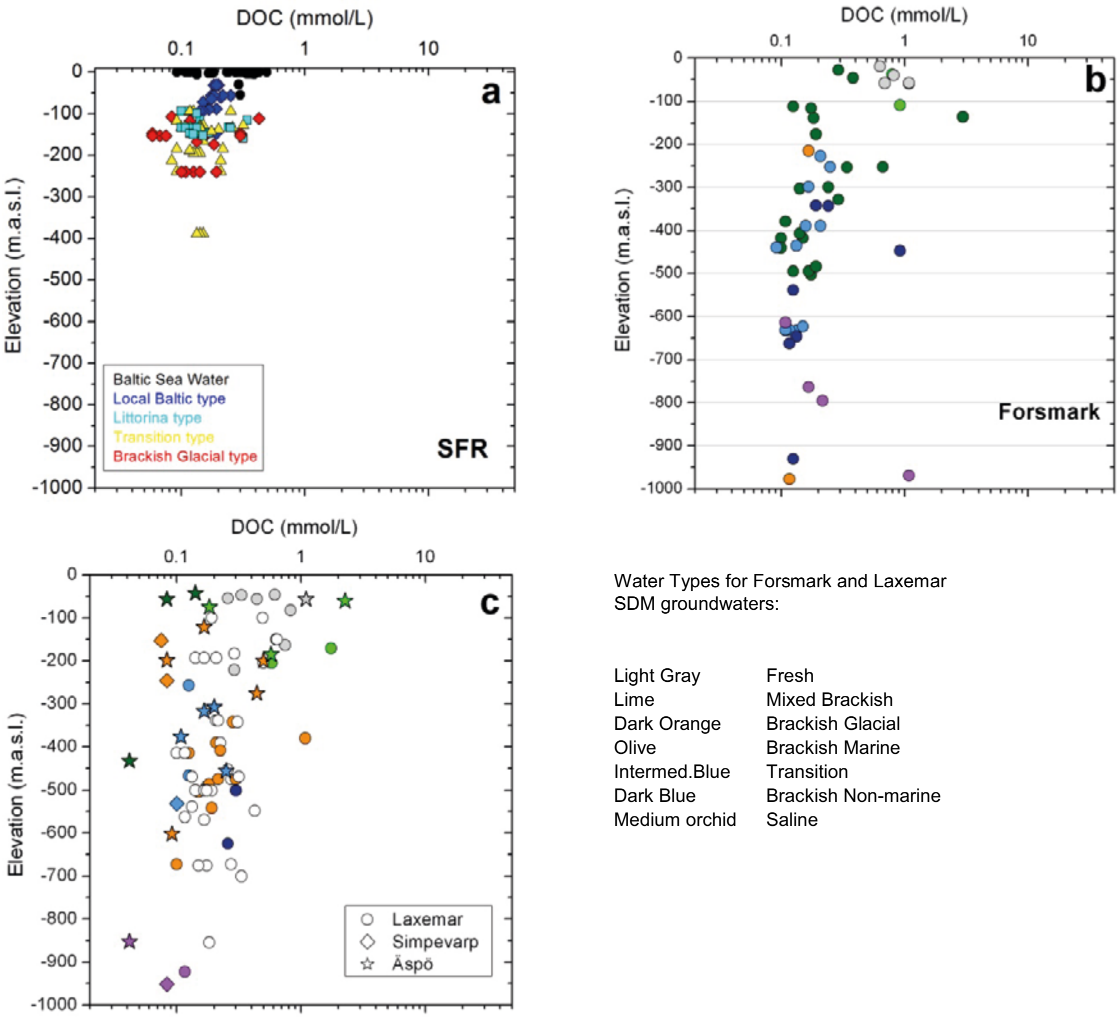
[12] The contents of TOC (analysed in unfiltered samples) and DOC (analysed in filtered samples) in the SFR, Laxemar and Forsmark groundwaters are usually very similar (Nilsson et al. 2010, Gimeno et al. 2010). Only locally TOC was found to be significantly greater than DOC. Thus, only the values of dissolved organic carbon will be discussed in this Appendix.



Water Types for Forsmark and Laxemar SDM groundwaters:

Light Gray	Fresh
Lime	Mixed Brackish
Dark Orange	Brackish Glacial
Olive	Brackish Marine
Intermed.Blue	Transition
Dark Blue	Brackish Non-marine
Medium orchid	Saline

Figure B-1. *Depth distribution of dissolved organic carbon (DOC) in the SFR (a) Forsmark SDM (b) and Laxemar-Simpevarp-Äspö SDM (c) areas. Samples are coloured by water type as indicated in the legends (Laaksoharju et al. 2008, 2009, Gimeno et al. 2011). Open symbols in plots b and c correspond to samples for which a water type has not been defined.*

Table B-1. Maximum, minimum and mean values of DOC for the SFR groundwaters. Concentrations are expressed in mg/L and mmol/L (between brackets). The number of samples analysed for DOC is also indicated.

	Min. value	Max. value	Mean	Number of samples
Baltic type waters	1.7 (0.14)	3.0 (0.25)	2.17 (0.18)	17
Littorina type waters	1.2 (0.1)	4.1 (0.34)	1.87 0.16)	22
Glacial type waters	0.7 (0.06)	5.1 (0.42)	1.80 (0.15)	17
Transition type waters	1.0 (0.08)	3.8 (0.32)	1.73 (0.14)	42
All SFR groundwaters	0.7 (0.06)	5.1 (0.42)	1.85 (0.15)	98

At the shallower and more hydraulically active levels (down to 200 m depth), DOC contents show significant variations and the highest value, up to around 35 mg/L (2.92 mmol/L), is observed in a brackish marine groundwater. However, the rest of the values at these depths are lower than 12.2 mg/L (≈ 1 mmol/L). Deeper down (below 200 m depth), DOC values are between 1 and 5 mg/L (0.08–0.42 mmol/L) except for a few cases with higher values (around 12 mg/L ≈ 1.0 mmol/L) in some brackish non marine to saline groundwaters (Figure B-1b).

A similar situation is found at the Laxemar and Äspo areas. DOC concentrations in the near-surface groundwaters from Laxemar range from 4 to 22 mg/L (0.33 to 1.83 mmol/L) although 97% of the data are below 15 mg/L (1.25 mmol/L; Tröjbom and Söderbäck, 2008). Fresh and shallow groundwaters in the upper bedrock (<100 m depth) show even lower concentrations than in the Forsmark site, from 3 to 9.5 mg/L (0.25 to 0.8 mmol/L; Figure B-1c). The highest values, up to around 20 mg/L (1.67 mmol/L) at Laxemar and 26 mg/L (2.17 mmol/L) at Äspö, occur in some mixed brackish type groundwaters down to 200 m depth (Figure B-1c). However, most of the values at these depths are lower than 12 mg/L (1 mmo/L). Below 200 m depth and with only one exception, DOC concentrations are below 4.8 mg/L (0.4 mmol/L; Figure B-1c).

The review performed by Gimeno et al. (2010) about the DOC (or TOC) values at depth in crystalline systems (see Table 5-1 in Gimeno et al. 2010) indicated that, in general, they show concentrations from 1 to 6 mg/L (0.08 to 0.5 mmol/L). This is true even at depths as great as 2.8–3.3 km in the mines from South Africa or in deep groundwaters where only autotrophic metabolisms are active like in the Mponeng Mine (Lin et al. 2006, Chivian et al. 2008). Thus, this range (1–6 mg/L or 0.08–0.5 mmol/L) could be considered as the "usual values" in groundwaters from crystalline systems. However, it was also found that some systems, like the Grimsel Test Site (glacial derived groundwaters) or the Henderson Mine, show very low DOC concentrations (below 0. 6 mg/L or 0.05 mmol/L).

In this context, the reason for the occasionally increased values found in the Laxemar and Forsmark sites below 200 m depth (even in some of the deepest and oldest saline groundwaters in the Forsmark site; Figure B-1b) or for the high values found in some brackish-marine groundwaters is not clearly known. Contamination during drilling/sampling, new routines for cleaning the equipment, natural sources such as asphaltite or autotrophic metabolisms, Littorina Sea influences, etc have been discussed (Laaksoharju et al. 2008, 2009). Knowing that the analysis of organic matter in deep groundwaters is a complicated task due to sampling and analytical reasons, these highest DOC values need to be handled with caution. New data from the monitoring programme have not clarified the long term behaviour of DOC yet (Tullborg et al. 2010). Similar problems with the DOC contents have been found at Olkilouto (Finland) and the data have been considered unreliable due to organic contamination of the sampling equipment (Pitkänen et al. 1999, 2004).

In any case, the SFR groundwaters do not show this type of problems (at least, at the magnitude observed in Forsmark, Laxemar or Olkiluoto sites) and the DOC contents are in the "usual range", even in the groundwaters affected by the present intrusion of the Baltic Sea. Furthermore, with the available data on DOC contents, it appears that the SFR facilities have not promoted meaningful DOC contamination.

B2 DOC contents proposed to be used for the different climate domains

The climate domains considered in this assessment are temperate, periglacial and glacial. As in the main text, two possible situations will be considered for the *temperate domain*: the case of the site being submerged by the Baltic Sea (as today) and the case of the site above the sea level not covered by seawater due to the isostatic uplift. In the first case, an inflow of brackish groundwater (similar to the situation at present) will dominate. In the second case, land uplift will have proceeded so far that the groundwater flowing into the repository will be fresh (non-saline) having originated from recharge areas inland.

The *periglacial domain* is defined as regions that contain permafrost. The groundwaters expected to be around the repository during this domain are considered to be similar to the waters during the temperate domain when the repository is not covered by the sea. Within this climatic domain, the site may also, at times, be submerged under the sea and as there are no data about the effects of freeze-out under this situation, the proposal here is that groundwaters would be similar to the brackish groundwaters proposed for the temperate domain submerged under the sea, although this matter needs further studies.

Finally, for the *glacial domain,* the repository will be located beneath an ice sheet and inflowing meltwater of low salinity will saturate the repository. The proposed compositions for all these groundwaters can be seen in Chapter 4.

Temperate climate domain (repository submerged under the sea)

During this climate domain, the situation of the repository will be similar to the situation at present, with the SFR covered by the Baltic Sea, and the groundwater around the repository characterised as a brackish saline groundwater.

In this context, the overall range in the DOC contents found in the SFR groundwaters (from 0.7 to 5.1 mg/L or 0.06 to 0.42 mmol/L; Figure B-1a) with a mean value of 1.85 mg/L (≈ 0.15 mmol/L) could be proposed for this domain. This range is defined by the shallow groundwaters (<200 m depth; Figure B-1a) at the SFR where all compositional types are present (Baltic, Littorina, Glacial and Transition types). At shallowest levels (< 80 m depth), Baltic type groundwaters dominate and the DOC values show a narrower range (from 1.7 to 3.0 mg/L or 0.14 to 0.25 mmol/L; Table B-1) even with respect to the recharging Baltic seawaters near the SFR (Figure B-1a).

It could be argued that in other periods, also with seawater covering the repository site, larger amounts of organic matter would be expected in the marine recharge groundwaters, enhancing microbial activity at shallower levels. Presently, some of the shallow groundwaters (< 200 m depth) at the Forsmark and Laxemar sites with a high old-marine Littorina contribution have very high DOC concentrations (up to 35 mg/L or 2.92 mmol/L; Figure B-1b, c). However, other groundwaters with similar Littorina contributions have very low DOC contents and, as stated above, the origin of those high values could be associated to sampling problems.

Temperate climate domain (above the sea level)

During this domain, the climate will still be temperate but due to shoreline displacement, the repository will not longer be beneath the sea. Under these circumstances the groundwater flowing into the repository will be fresh (non-saline) throughout the period, with a low chloride content and originated from recharge areas (above the sea level, inland).

In order to select the DOC contents for the groundwaters in this domain, SFR data cannot be used as the repository is under the seafloor at present and no significant evidence of meteoric waters has been found. Therefore, near surface and fresh, shallow groundwaters from the Forsmark and Laxemar sites (exclusively derived from meteoric recharge) have been used for the assessment of this domain.

Near-surface groundwaters show a wide range in DOC contents at both sites, reaching values as high as 40 mg/L (3.33 mmol/L) in the Forsmark site and 22 mg/L (1.83 mmol/L) in Laxemar. However most of the analysed DOC values in this type of groundwaters are below 16 mg/L (1.33 mmol/L). Fresh and shallow (< 100 m) groundwaters show a narrower range, between 6 and 13 mg/L (0.5 to 1.08 mmol/L; Figure B-1b) in the Forsmark site and between 3 to 9.5 mg/L in the Laxemar (0.25 to 0.8 mmol/L; Figure B-1c). As stated above, the decrease in DOC contents from the near surface to the shallow groundwaters is consistent with the effects of microbial activity during the infiltration of the meteoric waters.

Thus, the DOC values in the fresh, shallow groundwaters from the Forsmark site (from 6 to 13 mg/L or 0.5 to 1.08 mmol/L) can be considered the most suitable for this assessment due to its proximity to the SFR. The DOC values in the fresh, shallow groundwaters from Laxemar (from 3 to 9.5 mg/L or 0.25 to 0.8 mmol/L), a more hydraulically active system, could be alternatively proposed when considering the possibility of a very long temperate climate domain (as in the *"extended global warming climate case"*).

Periglacial climate domain

During this domain the site may be above the sea level or, at times, be submerged under the sea; and as explained in the main text (see Section 4.2), there is very little information concerning the chemical characteristics of groundwaters related to permafrost conditions.

The scarce available data suggest that the permafrost related groundwaters around the repository would show hydrochemical characters similar to the fresh groundwaters during the temperate period (when the repository is not covered by the sea). During the periglacial domain the climate will be colder than during the temperate domain and, although the microbial activity may persist at these low temperatures (Hallbeck 2009, Sidborn et al. 2011 and references therein), neither the intensity of the biological activity in the surface nor DOC contents in the recharge waters are expected to increase. Therefore, the DOC contents for these groundwaters may be considered to be similar to the waters during the temperate domain (when the repository is not covered by the sea) and then:

- For the case with temperate and periglacial periods not extending for more than approximately 20–40 thousand years, values in the fresh, shallow groundwaters from the Forsmark site (from 6 to 13 mg/L or 0.5 to 1.08 mmol/L) can be considered.
- For the climatic case with temperate and periglacial periods extending for more than approximately 40 thousand years, the DOC values in the fresh, shallow groundwaters from the Laxemar site (from 3 to 9.5 mg/L or 0.25 to 0.8 mmol/L) can be proposed.

Within this domain, if the site is submerged under the sea, the DOC content in the groundwaters around the repository is proposed to be similar to those in the brackish groundwaters during the temperate domain (submerged under the sea), that is, from 0.7 to 5.1 mg/L (or 0.06 to 0.42 mmol/L).

Glacial climate domain

During this climate domain, permafrost and glaciation will affect the composition of the groundwaters reaching the repository. When the repository is located beneath a warm-based ice sheet, the inflowing meltwater will result in low salinity groundwater conditions. Moreover, the input of organic carbon with the recharging groundwater is expected to be low, because photosynthetic production of organic carbon will be reduced (SKB 2010b, Salas et al. 2011). However, additional sources of organic carbon may still remain related to:

- Microbial communities both in supraglacial (the surface ice areas) and in subglacial (at the ice-bed interface) environments (e.g. Hodson et al. 2008, Bhatia et al. 2010 and references therein) that may be still active.
- Previously overridden soil and vegetation at the base of ice sheets or glaciers (e.g. incorporated into glacial sediments and basal ice – debris-rich ice formed at that base-) that might be mobilised as DOC by the meltwaters in the subglacial environment or during deglaciation (Skidmore et al. 2000, Barker et al. 2006, Bhatia et al. 2010).

Although it was thought that glacial environments were devoid of life, specially, in the subglacial zones, recently an increasing number of studies evidence the presence of microbial communities at surface and beneath glaciers and ice sheets. Photosynthetic and heterotrophic microorganisms are active at surface (Hallbeck 2009, SKB 2010b) whereas aerobic and anaerobic microorganisms constitute the subglacial microbial communities. These subglacial comunities play an active role in mediating dissolution and oxidation of minerals in rocks and sediments beneath ice masses (Skidmore et al. 2005, Boyd et al. 2011) and participate in the carbon cycle through oxidation of organic carbon stores beneath glaciers and ice sheets masses (Bhatia et al. 2010). Therefore, these biological activities may introduce organic carbon in the recharging glacial meltwaters and, at the same time, may control the amounts of DOC remaining in the groundwaters.

The existence of the active microbial communities at different parts of glaciers and ice masses has been reviewed and discussed in the context of recent performance assessment by SKB (e.g. Hallbeck 2009, SKB 2010b, Sidborn et al. 2011). However, the DOC concentrations in the meltwaters and ice of those microbiologically studied glaciated systems have not been evaluated. As they may provide some reference or, at least, orientative values for the waters in the glacial climate domain, a review of these works and their results is summarised in Table B-2.

Data from subglacial (basal ice and meltwaters) and supraglacial (ice, snow and meltwaters) environments have been included in the table. They are usually interconnected as supraglacial meltwaters, generated by melting of snow and ice in the surface of the ice sheets, may reach the ice-bed interface through crevasses and moulins and mix with the basal meltwaters (Skidmore et al. 2000, Barker et al. 2006). In summary, the data considered here correspond to the supraglacial environment (including snow and meltwater samples) and to the subglacial environment, which includes not only the subglacial meltwaters but also the subglacial ice and, specifically, the basal ice.

Table B-2. DOC values found in water and ice samples from different ice sheets, glaciers and glaciated areas around the world. Glacial environments are simplified in supraglacial and subglacial ones. DOC contents are expressed both in mg/L and µmol/L as the more frequent units used in the reviewed works. Number of samples involved in the concentration ranges is indicated between brackets.

Location	Type of samples	Environment	DOC	References
Greenland Ice Sheet	Samples at two locations along the western margin of Greenland from a meltwater pond (supraglacial) and from a subglacial stream exiting at the base of glacier 'N'	Supraglacial meltwater	0.192 mg/L or 16.0 µmol/L (n = 1)	Bhatia et al. (2010)
		Subglacial meltwater	0.18–0.61 mg/L or 15–51 µmol/L (n = 3)	
Victoria Upper Glacier (Antarctica)	Samples of basal ice	Subglacial basal ice	1.78–46.66 mg/L or 148.3–3888.3 µmol/L	Barker et al. (2006)
Alpine glaciers in the Taylor Valley (Antarctica)	Analyses from snowpits that represent snow accumulation from the 1990s	Supraglacial snow	< 0.096 mg/L or < 8 µmol/L	Lyons et al. (2007)
Robertson Glacier (Canada)	Samples from two main subglacial streams	Subglacial meltwaters	0.22–0.399 mg/L or 18.3–33.3 µmol/L (n = 4)	Boyd et al. (2011)
John Evans Glacier (Canada)	Samples from supraglacial (drysnow, seasonal meltwater on the glacier's surface and several streams) and subglacial (basal ice and melt waters from the glacier snout)	Supraglacial snow	0.38–1.35 mg/L or 31.7–112.5 µmol/L. Mean 1.0 mg/L or 83.3 µmol/L (n = 3)	Bhatia et al. (2006)
		Supraglacial waters	0.3–3.4 mg/L or 25 –283.3 µmol/L. Mean 1.2 mg/L or 100 µmol/L (n = 11)	
		Subglacial waters	0.3–3.7 mg/L or 25–308.3 µmol/L. Mean 1.7 mg/L or 141.7 µmol/L (n = 6)	
		Basal ice	0.6–244 mg/L or 50–20,333 µmol/L. Mean 62 mg/L or 5,166 µmol/L (n = 5)	
	Samples from supraglacial and subglacial meltwaters	Supraglacial	0.114–0.47 mg/L or 9.5–39.2 µmol/L (n = 35)	Barker et al. (2006)
		Subglacial	0.124–0.427 mg/L or 10.3 to 35.6 µmol/L (n = 48)	
	Glacier ice and basal ice samples, supraglacial and subglacial water samples	Supraglacial waters	0.11–0.47 mg/L or 9.16–39.2 µmol/L (n = 54)	Skidmore et al. (2005)
		Subglacial waters	0.12–0.43 mg/L or 10–35.8 µmol/L (n = 47)	
		Glacier ice	0.29 mg/L or 24.2 µmol/L (n = 1)	
		Basal ice	1.2 mg/L or 100 µmol/L (n = 1)	
Outre Glacier (Canada)	Samples from supraglacial and subglacial meltwaters and of basal ice	Supraglacial	0.111– 0.328 mg/L or 9.2–27.3 µmol/L (n = 3)	Barker et al. (2006)
		Subglacial	0.057–0.175 mg/L or 4.7–14.6 µmol/L (n = 72)	
		Basal Ice	0.301–0.305 mg/L or 25.1–25.4 µmol/L (n = 2)	
Bow Glacier (Canada)	Bow Glacier outflow during three summers	Subglacial waters	0·14 to 0·77 mg/L or 11.7–64.2 µmol/L (n = 61)	Lafrenière and Sharp (2004)
Green Lake 5 rock glacier (USA)	Time series analysis at the outflow of the glacier	Subglacial waters	0·71 to 1·1 mg/L or 59.2–91.7 µmol/L (n = 17)	Williams et al. (2007)
Gulf of Alaska (USA)	Samples from stream waters in 11 coastal watersheds.	Supraglacial waters	0.6–2.2 mg/L or 50–183.3 µmol/L (n = 11)	Hood et al. (2009).
Bench Glacier (Alaska, USA)	Subglacial stream samples, basal ice samples and supraglacial meltwaters	Overall range	0.4 –7.4 mg/L or 33.3–616 µmol/L	Skidmore et al. (2005)

In general, most of the reviewed DOC contents in supraglacial snow and meltwaters are lower than 0.5 mg/L (≈ 42 µmol/L; see Table B-2) although some samples may reach values up to 3.4 mg/L (Bhatia et al. 2006). In contrast, DOC contents in the subglacial environment seem to be much more variable (low in the meltwaters and high in the basal ice) reaching values up to 244 mg/L.

The main reason for this variability lays on the fact that the basal ice is chemically and physically distinct from the overlying glacier ice because it includes meaningful amounts of sediment and it is formed by processes that occur at the glacier bed. The degree of contact between source waters, rock material, and organic carbon prior to formation of the basal ice layer, influences the chemistry and heterogeneity of the basal ice samples (Skidmore et al. 2000, Bhatia et al. 2006). For example, from the five basal ice samples collected in the John Evans Glacier, two of them provide very high DOC values (63 and 244 mg/L) whereas the others show contents below 1 mg/L (Bhatia et al. 2006) and something similar happens in the samples at the Victoria Upper Glacier (Barker et al. 2006).

On the other hand, subglacial meltwaters (even those related to the aforementioned basal ice samples; Table B-2) show lower contents, usually below 1 mg/L (≈ 84 µmol/L) and thus, much more similar to the range found in the meltwaters from the supraglacial environment.

The available data is still limited and the reason for the differences between the basal ice and the subglacial meltwaters is not clear yet. But the low DOC concentrations found in the subglacial meltwaters supports the assumption of low organic carbon in the glacial systems (e.g. Hood et al. 2009). Therefore, a range of 0.3 to 3.7 mg/L, covering the whole range of all the subglacial waters (and corresponding to the range of those from John Evans Glacier; Table B-2) could be considered for the DOC contents in groundwaters at the glacial climate domain. Apart from this, it is important to indicate that only a part of the total DOC contents is bioavailable (e.g. metabolically suitable; see Gimeno et al. (2010) and references therein) and, thus, the effective DOC amounts for microbial degradation would be even lower. In some glacial environments bioavailable DOC represents less than 60% of the total DOC (e.g. Hood et al. 2009).

Therefore, given the uncertainty associated to DOC quantification and the provisional low expected values, it is recommended to assume that DOC contents in the recharge waters do not contribute to microbial activity. This assumption has been considered in PA calculations related oxygen intrusion (Guimerà et al. 2006, Spiessl et al. 2008, Sidborn et al. 2010) where microbial activity and degradation of organic material have been pessimistically (or realistically) neglected.

Appendix C

Data Table used for this work. Excel file structure and contents

The excel file delivered by SKB to be used for this work is stored in the data base called "subversion" (TortoiseSVN version 1.8.3-1; svn.skb.se) with the name "SR-PSU_chemistry.xlsx". This file consists of two excel sheets: info and data. The first one indicates briefly the meaning of the columns that are shown in the second one, the second sheet contains the data (9,097 rows). These data include all the water samples (groundwater and surface water) collected during the site investigations in Forsmark, Laxemar and SFR. Additional data from wells, experiments, different controlling sampling campaigns and the ulterior monitoring programmes carried out in these sites, have also been considered. Finally, a broad set of regional data from private wells in northern Uppland (defined by N: 6633169 - 6725589, E: 627152 - 733165, Sweref99TM) are also included.

To perform the selection of waters that has been presented in this report, this original excel file was separated into several data sets. The final excel file is named "SR-PSU_HydroChemistry_Modelling_Table.xlsx" and the explanation of its structure and the content of the different subtables is the aim of this Appendix.

The name and content of these subtables is the following:

- 1_Data(mgL). This table contains the same information as the original table (SR-PSU_Chemistry.xlsx) but the data are shown in mg/L (instead of µg/L as in the original file). The number of samples included in this table (as indicated above) is 9,097.
- 2_Data(mgL)WaterTypes+Category. Based on the information from the SDM work (Forsmark, Laxemar, SFR, Sulphide), the category of the samples has been included. Additionally, several duplicated rows have been removed. The total number of samples is 9,053 and they have been sorted by the type of water and the site. The ID code corresponding to each sample in the original table (1_Data) and the ID in the Sicada databaseare also included in the first columns.
- 3_ForRefWatAllGW+NewComplete. Based on Table 2 but only groundwaters (near surface of deep) with complete data (for major ions). Empty samples have been moved to Table 5 (1,132). Samples without data for any of the major ions have been moved to Table 6 (1,077). Samples from Lakes, Streams, Sea Water and Precipitation have been moved to Table 7 (3,462).This table contains 3,382 samples. It is the table used for statistical calculations in this work when all the samples from each group are used.
- 4_ForRefWatGWRep+NewComplete. Based on Table 3 but only the samples considered representative during the Site investigations. Representative samples from Monitoring programmes have been removed. All the non representative samples have been moved to Table 8. This table contains 1,543 samples. It is the table used in this work for statistical calculations when only the representative samples from each group are used.
- 5_Empty samples. Samples without data for any of the major ions (except some bicarbonate data). There are 1,132 samples and they have been removed from Table 2.
- 6_Incomplete Samples. Samples without data for some major ions (all anions or all cations or the main elements, Cl, Na, Ca). There are 1,077 samples and they have been removed from Table 2.
- 7_LakesStreamSeaWatPrecip. There are 3,462 samples taken in the surface, including Lakes, Streams, Sea Water and Precipitation. They have been removed from Table 2. There are 872 samples from lakes, 1,414 from streams, 911 from the sea and 265 samples from precipitation.
- 8_NonRepr_NonUsedGWSDM. Samples removed from Table 4 as they are not considered representative. They correspond to low category samples from the SDM (category 5) or to time series, some monitoring samples taken after the SDM and additional samples not used in SDM (drilling water, process control, experiment water, returned water...). The total of samples in this table is 1,839: 686 groundwater samples and 151 near-surface groundwaters from Forsmark SDM and SFR (84 groundwater samples), 634 groundwaters and 143 NSGW from Laxemar, 101 samples corresponding to special sampling procedure (drilling, etc), 92 samples from sediment porewaters in Forsmark SDM dataset and Laxemar and 32 samples from the monitoring programme.

There are two initial sheets in the Excel file with a brief explanation of the data sets contents and a description of the columns included in the data sets.

- Original Info: Contains the list of the columns included in the data tables together with some brief descriptions of their contents.
- Additional Info: Specifically prepared for this file, contains a brief description of the file and the modifications performed during this work.

And finally, there is a last sheet with the specific information about the water types for all the samples included in the original data set ("Sample Types Explanation"). This table includes the different names of the samples and subsamples, sampling methods and references when available.

The same structure is shown for the different data set tables. The columns cover a thorough information for each sample, from their identification codes, location, date, additional information about the type of sample, the field and laboratory physicochemical measurements (pH, Eh, T, conductivity) and the whole chemical analyses (major, minor, trace elements, isotopes, microbes and gasses if available).