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Assessment of groundwater salinity evolution at repository depth and especially the impact of dilute water infiltration

Main Review Phase

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SSM perspektiv

Bakgrund

Strålsäkerhetsmyndigheten (SSM) granskar Svensk Kärnbränslehantering AB:s (SKB) ansökningar enligt lagen (1984:3) om kärnteknisk verksamhet om uppförande, innehav och drift av ett slutförvar för använt kärnbränsle och av en inkapslingsanläggning. Som en del i granskningen ger SSM konsulter uppdrag för att inhämta information i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Syftet med detta projekt är att göra en oberoende utvärdering av grunden för SKB:s analys av salthaltsutveckling och avgöra om det finns några skäl för att en större andel av deponeringshålen skulle kunna bli påverkade av grundvatten som är utspädda till en sådan nivå att erosion av bufferten kan påbörjas.

Författarens sammanfattning

Grundvattensammansättningen in deponeringshål i slutförvaret kommer successivt att spädas ut med tiden på grund av topografiska förhållanden och klimatutvecklingen vid Forsmarkplatsen. Detta är en fråga med betydelse för slutförvarets långsiktiga säkerhet eftersom mycket utspädda vatten kan destabilisera kompakterad bentonit och erodera bufferten, vilket leder till advektion av sulfidhaltiga grundvatten till kapselytan. SKB:s slutsats i SR-Site är att endast ett mycket litet antal deponeringshål skulle potentiellt påverkas av advektiva och utspädda grundvatten som leder till bufferterosion, vilket beror på de hydrogeologiska egenskaperna för den begränsat uppspruckna berggrunden och processerna för vatten-berg reaktioner för den ytliga infiltrationen, hydrodynamisk blandning och utbyte med porvatten i bergmatrisen. Denna ståndpunkt grundar sig på resultat från en komplex modellering av grundvattenflöde och salttransport. Konceptualisering och utformning av modellerna inklusive de aspekter som beskriver spricknätverket, kräver oundvikligen olika antaganden och förenklingar. SKB har utvärderat effekterna av dessa genom känslighetsanalyser och finner att modellering av salthaltutveckling är tillräckligt robust.

Den långsiktiga utvecklingen av grundvattnets salthalt på förvarsdjup vid Forsmark kommer att kontrolleras av olika egenskaper hos berggrunden och vattensammansättningar i den omgivande miljön. Bergrundsegenskaper som kommer att påverka penetrationen av utspädda vatten i deponeringshål inkluderar sprickstrukturer i berget, transmissivitet, konnektivitet, dispersion och matrisdiffusion. Graden av utspädning kommer att kontrolleras av sammansättningen av nuvarande grund- och porvatten i sprickor och bergmatris, av infiltrerande vatten under kommande tempererade och glacial klimat samt av de processer som modifierar och blanda dessa komponenter. SKB har gjort alla rimliga försök att karakterisera sammansättningen av grund- och porvatten i nutid och för initialtillståndet för 10 000 år sedan. Min bedömning är att kunskapsnivå om grundvattensammansättningar, distribution och källor till de olika komponenterna i grundvatten i allmänhet är tillräcklig.

Modellen har kalibrerats med hjälp av statisk bearbetning av testdata och grundvattensammansättningar, vilket har minskat vertikal hydraulisk konduktivitet med en storleksordning. Kalibrering har varit möjligt endast för den grundare delen av systemet, över -400 m, eftersom det finns mindre data på djup mot förvarsdjup. Denna metod för att för att karaktärisera storskaliga flödes- och transportegenskaper är så robust som rimligen kan uppnås.

Det finns flera aspekter av modelleringen av salthaltutveckling för vilka rapporteringen är otydlig, såsom valet av referenssammansättning för utspädd vatteninfiltration. Det ger intrycket att modell gjordes med en grad av lämplighet för detta särskilda ändamål. Enligt min bedömning är tillvägagångssättet i grunden robust och motiverat, men beskrivningen av det som gjorts är svåra att följa. Jag drar slutsatsen att det finns relativt stora återstående osäkerheter i ECPM representationen av inträngning av utspädda grundvatten ner mot förvarsdjup, även om dessa osäkerheter sannolikt innebär att resultatet av modelleringen är pessimistiskt.

Simuleringar av infiltration av utspätt vatten under den tempererade perioden för basfallet har till största delen varit för tidsperioden 10 000 år. Modellering för scenariot för global uppvärmning med en löptid på 60 000 år är däremot mindre tillfredsställande eftersom endast lite information har tillhandahållits. Den mycket begränsade grafiska illustrationen av resultat gör att endast en förenklad och otillfredsställande jämförelse mellan modellresultat för de två olika tidsramarna kan göras.

Regional-modellering av utvecklingen av salthalt under en istid har gjorts av SKB på ett likartat sätt som för den tempererade perioden. Den ursprungliga salthalten i grundvattnet på förvarsdjup i slutet av den tempererade perioden och i början av en istid har tilldelats ett värde 3 g/L TDS, vilket också är salthalten för porvatten i bergmatrisen. Modellering av salthalt för den långvariga tempererade perioden på 60 000 år tyder på att salthalten förmodligen skulle vara mycket mindre än 3 g/L, så effekterna av en lägre initial salthalt borde ha beaktats. Å andra sidan är det en mycket utspädd sammansättning av glacialt smältvatten som förutsätts i modellen. Dessutom ingår inte reaktioner med mineral i berggrunden vid beräkning av salthalten med evolutionsmodellen. Detta innebär att den regionala-modell av utspädd vatteninträngning under en istid är sannolikt är pessimistisk. Ett antal pessimistiska scenarier och tidsramar har även modellerats med infiltration under förhållanden med en fullständig nedisning för en period med längre varaktighet än 100 000 år. En annan modellvariant har antagit glaciala förhållanden för 25 % av de 120 000 år som motsvarar varaktighet hos nästa glaciationscykel. Dessa ”värsta fall” som beaktats vid beräkningsarbetet ger ett tillfredställande belägg för att säkerhetsanalysen är robust för osäkerheter.

Matrisutbyte kommer att vara mindre effektiv än den modellerade effekten på utspädda grundvatten om det förenklade antagandet att hela bergmatrisen är tillgängligt för diffusivt utbyte är ogiltigt, eller om värdena för diffusivitet för lösta ämnen i bergmatrisen eller för flödesvätt yta för sprickor har överskattats. Osäkerhet i parameterisering av dispersion för ECPM modellen betyder att graden av utspädning på förvarsdjup kan antingen vara över- eller underskattad. Känslighet på grund av dessa faktorer behöver förtydligas.

SKB konstaterar med hjälp av pessimistiska antaganden att endast ett deponeringshål kommer att exponeras för en kombination av flödeshastighet och utspädning i sådan omfattning att bufferten kommer att eroderas till en sådan nivå att advektiva förhållanden uppstår vid kapselytan. De antaganden som denna beräkning baseras på har inte förklarats. Det är oklart hur denna slutsats kan jämföras med de andra illustrativa beräkningarna av ”antal deponeringshål som blir utsatta för utspädda grundvatten”. Om resultaten från de olika illustrativa beräkningarna tolkas bokstavligt är sannolikheten för bufferterosion med utspädda grundvatten mycket låg. Ökat förtroende för denna slutsats skulle vara möjligt om SKB tydligare hade redogjort för argument som beräkningarna baserats på kopplat till giltigheten av DFN representation av spricksystemet och transmissivitet i närheten deponeringstunnlar. Trots detta kan dock den osäkerhet som följer av användning DFN modellen för modellering av vattentransport nära deponeringshål vara av underordnad betydelse i sammanhanget inflöde av utspädda grundvatten och risken för kemisk erosion av bufferten. Det beror på att mineraliseringen av grundvattnet på förvarsdjup med vatten som har spätts på grund av långvarig infiltration av meteoriskt eller glacialt smältvatten är sannolikt högre än kriteriet för bufferten säkerhetsfunktion.

Sammanfattningsvis är min bedömning av hur SKB hanterat utveckling salthalt att det finns olika kvarvarande osäkerheter i det sätt som transport av lösta ämnen, blandning grundvattentyper och dämpning salthaltvariationer med matrisdiffusion har modellerats och begränsats. Dessa osäkerheter kan potentiellt orsaka betydande variationer i det mönster av modellerad salthaltutveckling som funktion av tiden på förvarsdjup och runt deponeringshåls positioner. Med tanke på den särskilda gränsen kopplad till jonstyrka på <4 mM för utspädning för att bli betydande i fallet bufferterosion är min bedömning att det är mycket osannolikt att deponeringshålspositioner skulle exponeras för sådana markant utspädda inflöden.

Projektinformation

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Aktivitetsnummer: 3030012-4066

SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) reviews the Swedish Nuclear Fuel Company's (SKB) applications under the Act on Nuclear Activities (SFS 1984:3) for the construction and operation of a repository for spent nuclear fuel and for an encapsulation facility. As part of the review, SSM commissions consultants to carry out work in order to obtain information on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

The objective of this assignment is to make an independent assessment of SKB's basis for salinity evolution and determine if there are any reasons why a larger proportion of the deposition holes may be affected by dilute water infiltration to the extent that buffer erosion may be initiated.

Summary by the author

Groundwater compositions entering deposition holes in the repository will be progressively diluted over time because of expected changes of topographic and climatic conditions at Forsmark. This is a long-term safety issue because very dilute water could destabilise compacted bentonite and erode buffer, leading to advective movement of sulphide-containing water to the canister surface. SKB's position in SR-Site is that the hydrogeological properties of the sparsely-fractured bedrock and the processes of water-rock reaction in shallow infiltration, hydrodynamic mixing and exchange with pore waters in rock matrix will be such that only a very small number of deposition holes would potentially suffer advective dilute water conditions leading to buffer erosion. This position is based on the results of complex modelling of groundwater flow and salt transport. Conceptualisation and formulation of the models, including those describing the fracture network, inevitably require various assumptions and simplifications. SKB has assessed the impact of these by sensitivity analyses and finds the forecasts of salinity evolution to be adequately robust.

Evolution of groundwater salinity at repository depth in the long term at Forsmark will be controlled by various bedrock properties and environmental water compositions. Bedrock properties that will influence the penetration of dilute water into deposition holes include fracture patterns, transmissivity, connectivity, dispersivity and matrix diffusivity. The degree of dilution of that water will be controlled by compositions of present groundwaters and pore waters in fractures and rock matrix and of infiltrating waters during future temperate and glacial climates and by the processes that modify and mix these components.

SKB has made all reasonable attempts to characterise compositions of groundwaters and pore waters at the present day and for the model initial state at 10,000 years ago. My assessment is that the level of knowledge of groundwater compositions, their distribution and the sources of the different water components is generally adequate. The model is calibrated against interference test data and groundwater compositions, reducing vertical hydraulic conductivity by an order of magnitude. Calibration has been possible only for the shallower part of the system, above 400 m, because data are less dense towards repository depth. This approach to large-scale flow and transport properties is as robust as can reasonably be achieved.

There are several aspects of the salinity evolution modelling, such as the choice of reference water composition for dilute water infiltration, where the report lacks clarity. It gives the impression that the modelling was done with a degree of ad hoc expediency. The approach is basically robust and justifiable, in my opinion, but the description of what has been done is difficult to follow. I conclude that there are relatively large remaining uncertainties in the ECPM representation of dilute water penetration towards repository depth, although these uncertainties probably mean that the results of the modelling are pessimistic.

Simulations of dilute water infiltration during the temperate period of the base case evolution have mostly been for 10,000 years. Modelling for the variant global warming scenario with duration of 60,000 years is less satisfactory with very little information being provided. The very limited graphical illustration of results allows only a simplistic and unsatisfactory comparison between model outputs for the two timescales.

Regional-scale modelling of salinity evolution through a glacial period has been done by SKB in a very similar way to the temperate period modelling. The initial salinity of groundwaters at repository depth at the end of the temperate period and at the start of a glacial period has been assigned a value of 3 g/L TDS, as also has the salinity of pore waters in the rock matrix. Modelling of salinity through the prolonged temperate period of 60,000 years indicates that it would probably be much less than 3 g/L, so the impact of a lower initial salinity on the model should have been considered. On the other hand, the very dilute composition of glacial melt water that is assumed plus the fact that the salinity evolution model does not include rock alteration reactions of melt water mean that the regional-scale model of dilute water penetration during a glacial period is likely to be pessimistic. A number of pessimistic scenarios and timescales have been modelled including infiltration under fully glaciated conditions for an extended timescale of 100,000 years. Another model variant has assumed glacial conditions for 25% of the 120,000 years duration of the next glacial cycle. These ‘worst case’ model calculations satisfactorily indicate that the safety analysis is robust to uncertainties.

If the simplifying assumption that the entire rock matrix is accessible for diffusive exchange is invalid, or the values for solute diffusivity of the rock matrix or for flow-wetted surface area of fractures have been overestimated, then matrix exchange will be less effective than modelled at attenuating dilute water. Similarly, uncertainty in the parameterisation of dispersion in the ECPM model means that the degree of dilution at repository depth could be over- or under-estimated. Sensitivity to these factors needs to be clarified.

SKB concludes, using pessimistic assumptions, that only one deposition hole will experience a combination of flow velocity and water dilution of such severity that buffer will be eroded to the point of reaching advective conditions at the canister surface. The assumptions implicit in this estimation have not been explained. It is unclear how this conclusion compares with the other illustrative calculations of 'number of deposition holes receiving dilute water'. Taking the various illustrations at face value, the probability of buffer erosion by dilute water is very low. There would be greater confidence that this conclusion is valid if SKB could make a clearer case for the validity of the DFN representation of fracturing and transmissivity around deposition tunnels on which the conclusion is dependent.

However, in the context of dilute water penetration to deposition holes and the consequent risk of chemical erosion of buffer, the uncertainties arising from the DFN treatment of water transmission into deposition holes may be of secondary importance. That is because the mineralisation of groundwater at repository depth, even water that has been diluted due to prolonged infiltration of meteoric or glacial melt water, is very likely to be higher than the criterion for the buffer safety function.

In summary, my assessment of how SKB have handled salinity evolution is that there are various unresolved uncertainties in the ways that solute transport, groundwater mixing and salinity attenuation by matrix diffusion have been modelled and constrained. These uncertainties could potentially cause substantial variability in the patterns of modelled salinity development through time at repository depth and around deposition hole positions. However, given the specific threshold of <4 mM for dilution to become significant with regard to buffer erosion, my judgement is that it is very unlikely that deposition hole positions would experience such significantly dilute inflows.

Project information

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Contents

1. Introduction

SSM's scope of work for this assignment states:

> "The groundwater salinity evolution near canister deposition holes is controlling the onset of buffer erosion. SKB arrives at the conclusion that a few % of the deposition holes will be subjected to groundwater sufficiently dilute to initiate buffer erosion. This also means that for the vast majority of deposition holes the buffer will remain intact. The objective of this assignment is to make an independent assessment of SKB's basis for their utilized salinity evolution in SR-Site. The most critical issue is probably if there are any reasons why the proportion of the deposition holes affected by dilute water infiltration (to the extent that buffer erosion may be initiated) may be larger than the one currently used in SR-Site and if so how much larger. Sufficiently dilute water is mainly related to glacial melt-water infiltrating at the surface, but very long periods of temperate conditions should also be analysed with the buffer erosion criterion in mind."

This report is an assessment of SKB's reporting for SR-Site, and in supporting documents, of the variant scenario of chemical erosion of buffer due to inflow of very dilute groundwater to deposition holes and thence in contact with buffer. SKB have established a criterion for salinity in terms of summed cation equivalent concentrations, $\Sigma q[M^{q+}]$, whereby a value of 4 mM should be exceeded to maintain stable buffer. The validity of this criterion is assumed to for this review.

My review of SKB's presentation on the topic and my assessment of SKB's approach and of its robustness for the safety case focus on two main aspects of the issue: (a) the modelling of salinity evolution and specifically of the progressive dilution of groundwaters down to repository depth, and (b) the modelling of inflows of more or less dilute groundwaters into deposition holes. The important considerations for salinity evolution are the initial and boundary conditions for water compositions and the processes that are involved: hydrodynamic mixing, diffusive exchange with pore waters, and hydrogeochemical reactions. The important considerations for flows at deposition hole scale are the stochastic representation of minor fracturing in the rock mass by a discrete fracture network (DFN) model, how that DFN might connect with deposition holes, and the solute transport processes that might modify water salinity.

Section 2 of this report comprises two main parts: a review and summary of SKB's presentation of this topic, and my detailed assessment of SKB's presentation and of the completeness and robustness of the approach to dealing with the topic. There is also a brief section discussing motivation of my assessment - the relevance of salinity evolution and groundwater inflows at deposition holes to the variant safety case scenario of chemical erosion of buffer and the criteria for assessing robustness. The sub-divisions of the two main parts of Section 2 generally deal with (i) what is known about present-day groundwater compositions, (ii) initial state assigned as the basis for forward modelling of salinity evolution, (iii) modelling of dilute water infiltration and salinity evolution through a temperate period, (iv) modelling of dilute water infiltration and salinity evolution through a glacial period, (v) modelling of dilute water flow and dilution at deposition hole positions, (vi) effects of water-rock reactions on groundwater compositions, and (vii) other considerations.
Section 3 is a summary of my overall assessment.

2. Groundwater salinity evolution and dilute water infiltration to repository depth

2.1. SKB's presentation

2.1.1. Present-day groundwater and pore water compositions

SKB's understanding of the compositions of groundwaters at Forsmark is based on data measured in water samples from shallow soil drillholes, percussion boreholes to intermediate depths, and cored boreholes to maximum of about 1000 m. Flowing water samples from bedrock in percussion and cored boreholes are essentially representative of groundwaters in transmissive fractures.

The target volume, which is located in the 'footwall' rock to the north-west of the major sub-horizontal deformation zone A2, is dominantly classified as domain FFM01. The 'hanging wall' rock, south-east of A2, is a hydraulic regime with greater bulk permeability due to a number of gently-dipping fracture zones. The gently-dipping fracture zones make a large contribution to the hydraulic conductivity of the bedrock at Forsmark but are sparse in domain FFM01. Because of the generally low hydraulic conductivity in this domain and the consequent difficulties in sampling, there are relatively few data for groundwater compositions in FFM01 around and below repository depth.

In addition to those data for groundwaters, data for chloride (Cl^-) concentrations in pore waters in matrix of intact rock have been measured experimentally in drillcore samples from a small number of the deep boreholes. These data for present-day compositions of groundwaters and pore waters have been used in various ways to support the modelling of salinity evolution and dilute water infiltration.

In the context of this assessment, present-day groundwater compositions, total salinity (Total Dissolved Solids, TDS), Cl^- concentration and stable isotopic ratio ($^{18}O/^{16}O$) plus concentrations of other solutes, are used to check and calibrate the regional groundwater flow and solute transport model. The regional model, which is an ECPM (equivalent continuous porous medium) model and is constructed with upscaled hydraulic properties from the DFN (discrete fracture network) model, is run forwards from an initial condition representing the groundwater system and composition at the end of the last glaciation, 10,000 years ago. This modelling of salinity evolution is described in more detail in the next section.

Groundwater compositions including pH and Eh are used as the basis for interpretative modelling of hydrogeochemical processes, i.e. reactions between water and minerals, both secondary minerals within fractures and primary minerals in unaltered rock matrix. The concentrations of major solutes and of some minor and trace solutes such as sulphide HS^-, have direct or indirect relevance to long-term performance of the engineered barrier system (EBS). These reactions are superimposed on hydrodynamic mixing of waters with different origins in accounting for the overall evolution of groundwater compositions.

It is important to understand that in considering the variations and future evolution of general groundwater mineralisation in terms of salinity, TDS, at Forsmark, the mixing of waters from different sources and with varying salinities is the predominant cause of salinity changes. The dominant cause of salinity in these groundwaters, Cl^- anion, cannot be derived from water-rock reaction (see section 2.1.6) because there are no chloride-containing minerals in the system. Solutes originating from water-mineral reactions have concentrations that are limited at low levels by solubility equilibria and therefore make a relatively minor contribution to total salinity.

SKB's presentation of measured groundwater compositions describes overall salinity variations, which are of most direct relevance to the present issue of dilute water penetration, and also categorises groundwater compositions in terms of brackish/saline water and the dominant origin of salinity, i.e. marine or non-marine.

Groundwaters to about 200 m depth in the shallow part of the target volume have dilute to brackish salinities, with Cl^- concentrations from low values up to around 5000 mg/L. Various lines of hydrochemical evidence indicate that these waters derive from Littorina (9500 to 2500 y ago) and Baltic (modern) seawaters, plus meteoric water infiltration that must post-date subaerial exposure of the surface about 2500 y ago.

Below about 200 m depth in the deeper regime of the target volume, groundwaters are brackish (2000-6000 mg/L Cl^-) down to about 300 m, whereas in the hanging wall of A2 these compositions extend to 600-700 m. These brackish waters are mostly derived from Littorina infiltration, according to SKB's interpretation of hydrochemical evidence such as Mg^{2+} and Br^- concentrations (SKB 2011, p 131). Penetration of Littorina water in the fracture domain, FFM01, in which the repository would be located, is 'restricted to ca. 300 m' (p 132).

Below about 300 m depth in the target volume, fracture domain FFM01, it was possible to collect only 3 reliable groundwater samples, presumably due to the low frequency of transmissive fracturing (SKB 2011, Figure 4-21, p 132). Therefore there is little information about spatial variability of groundwater compositions. Sampled groundwaters are brackish to saline with 7000-8000 mg/L Cl^-. These are interpreted as being non-marine and derived from salinity with ancient origin in the deep bedrock. One of the characteristics of this deep saline groundwater is that, as in other 'Shield' brines, the proportion of Ca^{2+} amongst the cations increases with depth. This is attributed to water-rock reaction.

There are rather more groundwater samples from deformation zones between 300-800 m depth. These have a larger scatter of Cl^- concentrations, mostly between 6000-9000 mg/L plus two outliers below 600 m with 14000-15000 mg/L (SKB 2011, Figure 4-21). No groundwaters were sampled below 300 m depth with Cl^- concentrations significantly more dilute than about 6000 mg/L and the trend in Figure 4-21 (SKB 2011) does not suggest any such anomalies.

Compositions of mobile groundwaters in fractures are buffered to some extent by diffusive exchange of water and solutes between fracture waters and pore waters in adjoining rock matrix. Direct analyses of pore water compositions are not possible but have been measured in the laboratory by an experimental technique that exchanges solutes by out-diffusion between a test water sample and drillcore in purpose-built equipment. Reaction between test water and rock could change concentrations of many solutes unpredictably, so only Cl^- and bromide (Br^-)

concentrations can be estimated from these tests with reasonable reliability. Stable isotope ratios of pore waters can also be analysed by a similar method.

Results for pore water compositions from these tests are available for a few drillcores. They indicate that porewaters in the footwall rock have lower Cl^- concentrations and higher $\delta^{18}O$ values than nearby groundwaters in fractures down to at least 650 m depth. Porewaters in the hanging wall rock down to about 200 m depth have compositions that are equilibrated with fracture waters. Below that the porewater Cl^- concentrations deviate in the same way as porewaters in footwall rock, but in contrast $\delta^{18}O$ values become lower relative to fracture waters. The porewater compositions are interpreted as indicating equilibration over long periods with dilute groundwater, in the former case very old pre-glacial water and in the latter case glacial water predating the last glacial cycle (SKB 2011, p 132).

2.1.2. Initial state for salinity evolution modelling from 10,000 years ago

Evolution of salinity in the Forsmark bedrock groundwaters is initially modelled from 10,000 years ago through to 10,000 years in the future (Joyce et al. 2010, Section 4). Thus the regional-scale model of salinity is in part a palaeo-hydrogeological model and in part a forecast of how the system will evolve in the future. The model has been calibrated by comparing the modelled present-day compositions with observed compositions, though the details of the procedure are not reported and are therefore rather unclear. The modelling is done in terms of hydrodynamic mixing of reference waters, so the initial state is also defined in terms of reference waters and the observed data are interpreted as proportions of reference waters.

The initial state for groundwaters in fractures at 10,000 years ago is defined in terms of the deep saline, glacial melt, and old meteoric reference waters (SKB 2011, Table 1, p 341; Follin et al. 2008, p 50; Follin et al. 2007, p 96). The ‘old meteoric’ reference water has the same composition as present-day meteoric water except that the HCO_3^- concentration is reduced to that of the deep saline reference water. It was introduced in the stage 2.2 modelling to create an initial condition, i.e. depth profile of groundwater compositions, which does not represent complete replacement of pre-existing water by glacial melt water at the end of the last ice age. It also adds into the modelled groundwater mixtures a component that is inferred from the compositions of pore waters (see below).

The qualitative definition of reference waters in Table 6-1 of Joyce et al. (2010, p 80) appears to have a typographical error in the composition of old meteoric reference water. It states that it has a ‘strong saline source’ and therefore high Cl- (>20,000 mg/L) and intermediate stable isotope composition (-12 to -11 ‰ δ18O). This is inconsistent with data from Follin et al. (2007, p 96) that are in Table 1. There is another typographical error in tabulating Ca, Mg, Na and K data for the meteoric reference water in Laaksoharju et al. (2008, Table 1-1).

An ‘old meteoric + glacial’ reference water, having the same composition as the glacial reference water except for a heavier stable isotope ratio, was proposed by Laaksoharju et al. (2008, Table 1-1, p 15) and Gimeno et al. (2008, Table 2-14, p 47) as shown in Table 1. This was not used in subsequent modelling and it seems that instead the ‘old meteoric’ reference has been used.

Table 1. Compositions of reference waters used in modelling of evolution of salinity and groundwater compositions at Forsmark (from Table 4-1 in Salas et al. (2010); also Table 3-14 in Follin et al. (2008) with 'old meteoric water' added according to Follin et al. (2007, p 96). Concentrations are in mg/L except TDS which is in g/L. Stable isotope ratios are in per mil.

Reference water	TDS	Na	K	Ca	Mg	HCO_3	Cl	SO_4	$\delta^{18}O$
Present-day meteoric water*	0.30[†]	274	5.6	41.1	7.5	466	181	85.1	-11.1
Littorina sea water	10.7[†]	3674	134	151	448	92.5	6500	890	-4.7
Glacial melt water	0.002	0.17	0.4	0.18	0.1	0.12	0.5	0.5	-21.0
Old meteoric water*	0.30[†]	274	5.6	41.1	7.5	14.1	181	85.1	-5.0
Deep saline water	77.7[†]	8200	45.5	19300	2.12	14.1	47200	10	-8.9
Old meteoric + glacial water^	0.002	0.17	0.4	0.18	0.1	0.12	0.5	0.5	-16.0

*Meteoric water compositions are 'altered' by initial water-mineral reaction in soil.

^The last line is an extra reference water, 'old meteoric+glacial', not used in modelling but reported in Laaksoharju et al. (2008, Table 1-1, p 15) and Gimeno et al. (2008, Table 2-14, p 47).

[†] TDS is estimated from Cl^- concentration with the formula TDS (mg/L) = Cl (mg/L) x 1.646 (Eqn 4-2 in Salas et al. (2010, p 32).

The assigned compositions of these reference waters are explained and justified in Gimeno et al. (2008). The composition for the present-day altered meteoric water is based on a shallow groundwater from percussion hole HFM09 at 17-50 m depth (Gimeno et al. 2008, p 32). The composition for Littorina seawater is based on an estimated maximum salinity of 12 ‰ and diluting seawater composition to this level of salinity (Gimeno et al. 2008, p 22). The composition for Holocene glacial melt water is based on that of melt waters from the Josterdalsbreen glacier in Norway (Gimeno et al., 2008, p 18). The composition of old altered meteoric water is identical to that for present-day meteoric water except for HCO_3^-, as explained above. The composition of deep saline water is that of a groundwater sample from 1631-1681 m depth in borehole KLX02 at Laxemar (Gimeno et al. 2008, p 11) except that SO_4^{2-} is given a low concentration of 10 mg/L based on the outcome of sensitivity testing by Monte Carlo computations (see below); this is the best approximation in the absence of such a highly saline deep groundwater sample from Forsmark.

The depth profile for the footwall rock domain (FFM01) at 10,000 years ago (Figure 1, left) is a binary mixture of glacial melt water and old meteoric water down to -400 m (-500 m for the hanging-wall domain) (Figure 1, left). Below -400 m, there is ternary mixing of glacial melt water with both old meteoric and deep saline reference waters down to -1100 m (-1800 m in the hanging wall) and then binary mixing of old meteoric water and deep saline water down to -1500 m (-2300 m in the hanging wall), below which groundwater is assumed to be 100% deep saline.

The replacement of some glacial water with meteoric water in the depth profile means that the stable oxygen and hydrogen isotopic ratios in the initial condition profile are slightly heavier than was previously assumed (Figure 3-64 in Follin et al. 2007, p 97).

The initial state for pore waters in the rock matrix is defined as 100% old meteoric water down to -400 m (-500 m in the footwall) (Figure 1, right). Below -400 m, there is binary mixing with deep saline composition down to -1500 m (-2300 m in the hanging wall). In other words, it is assumed that the pore waters are in diffusive exchange equilibrium with old meteoric water down to -400 m (or -350 m?) depth in footwall rocks at the end of the last glaciation (-500 m in the hanging wall). Below that to -1500 m (-2300 m in the hanging wall), pore waters are binary mixtures of old meteoric and deep saline compositions. The assumed initial condition for pore water compositions at 10,000 years ago in Figure 1 does not contain any glacial reference water, on the basis that there had been insufficient time for significant diffusive exchange between fracture and pore waters (Follin et al. 2008, p 52). However this was modified for SR-Site by superimposing on the initial condition shown in Figure 1 (right) diffusion of fracture waters into pore waters to avoid an unrealistic step-change between fracture water and pore water compositions at the start of modelling (Joyce et al. 2009, Appendix C, p 144). This is justified by the long period of intermittent glaciations during which such exchange would have occurred.

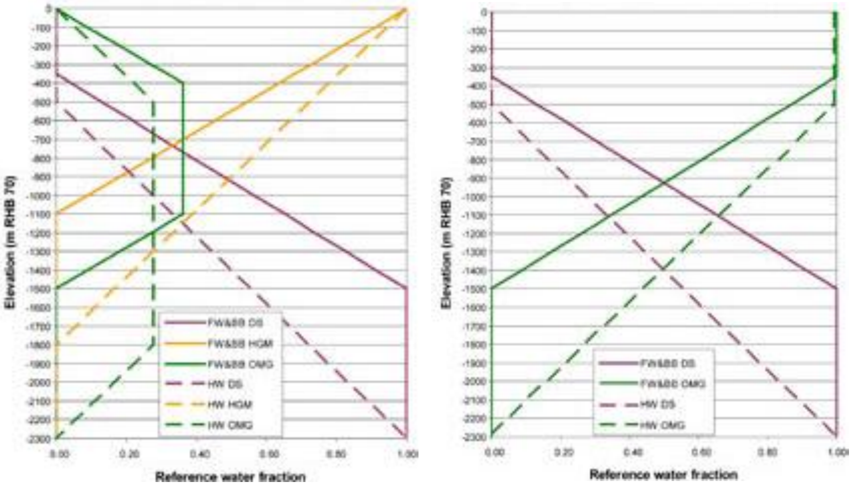

Figure 1: Initial state proportions of deep saline (DS) and glacial melt water (HGM) reference waters in fracture groundwaters (left) and matrix pore waters (right) in the footwall (FW) and hanging wall (HW) rock domains. [Extracted from Figures 3-63 and 3-67 in Follin et al. 2007; Figure 3-30 in Follin et al. 2008].

The hydrochemical boundary conditions applied to the model for salinity evolution vary with time, reflecting the topographic change due to land uplift, the consequent recession of the Baltic shoreline, and the forecast evolution of Baltic seawater salinity (Joyce et al. 2009, p 55). The top of the model grid, essentially the ground surface, is a recharge-discharge boundary through which Baltic seawater with salinity according to Figure 4-6 in Joyce et al. (2009, p 56), and/or meteoric water with the composition of the altered meteoric reference water, or glacial melt water infiltrate according to the modelled time and the corresponding assigned state of land uplift and climate. The sides and base of the model grid are assigned as no-flow boundaries.

The hydraulic boundary condition at the top boundary of the model is a fixed recharge amount of 150 mm/year in the recharge areas (Follin et al. 2008, p 53). A portion of this recharge is lost out of the discharge areas, so presumably the net recharge to the deep groundwater system is considerably lower than that. Future variations of precipitation are expected to vary substantially, especially in the early stages of global warming in the extended temperate climate variant scenario (SKB 2011, Vol 2, p 545). However the net effect on the amount of infiltration reaching repository depth is expected to be minor (p 547).

Sensitivity of Principal Component Analysis (PCA) calculations of the mixing proportions of reference waters to the compositions assigned to the reference waters has been investigated in Gimeno et al. (2008). Monte Carlo computations were used to calculate mixing proportions for a set of groundwater compositions when randomly selecting values for reference water compositions from a range of values around the assigned central values. For the deep saline, Littorina and altered meteoric reference waters, these ranges reflecting compositional uncertainties are very broad: i.e. 0.1 to 100,000 mg/L Cl^- for deep saline water, 3760 to 7000 mg/L Cl^- for Littorina, and 0.1 to 1000 mg/L Cl^- for altered meteoric water (Table 2-10 in Gimeno et al. 2008, p 38). It is unclear why such a wide range has been used for the deep saline reference water (perhaps this is a typographic error – the corresponding minimum Na^+ of 5000 mg/L is inconsistent). The range of compositions for altered meteoric water reflects conservatively the range of compositions of shallow groundwaters which, presumably, are already partially mixed with Baltic, Littorina or other brackish-saline water sources. The composition of the glacial reference water, except for stable isotopic ratios, was not varied in the Monte Carlo computations. These sensitivity tests did not include old meteoric reference water. Runs from the Monte Carlo computations that gave the lowest residuals in PCA were collected and plotted as histograms of frequency versus concentration for each solute.

The conclusions from the Monte Carlo modelling of sensitivity to assumed reference water compositions are that the concept of using these reference waters for interpreting palaeohydrogeological mixing of water components from distinct hydrochemical sources is fundamentally valid and that the PCA computations for inverse modelling of mixing are not generally sensitive to the exact compositions assigned to reference waters, although a few adjustments of specific solute concentrations have been made (Gimeno et al. 2008, p 46). From this conclusion, it was considered appropriate to use these reference waters compositions in palaeohydrogeological modelling and forwards evolution modelling of salinity and compositional evolution.

2.1.3. Modelling of dilute water infiltration and salinity evolution through the future temperate period

In the reference evolution of a repository at Forsmark, groundwater movements during the initial temperate period after closure are modelled at both site scale and repository scale until 10,000 years into the future. The duration of the temperate period in the reference evolution is around 30,000 years (SKB 2011, Fig 10-107, p 450). A variant scenario comprising an extended temperate climate due to global warming has also been modelled out to about 60,000 years into the future (SKB 2011, p 543). Details of that modelling and of any modelling for temperate conditions beyond the initial temperate period after closure, i.e. the next 7000 years, are not reported in the SR-Site Main Report (SKB 2011). The only reported results from the modelling are in Figure 10-32 and pages 547-548 (SKB 2011).

Hydrogeochemical evolution of groundwater compositions, i.e. change of groundwater chemical parameters by water-rock reaction as well as by mixing, has been modelled to 7000 years into the future (Salas et al. 2010; SKB 2010a). This will be summarised in Section 2.1.6.

Through the temperate period, uplift and shoreline regression cause increasing meteoric water infiltration and thus dilution of pre-existing brackish/saline groundwaters. During the period of repository construction and operation, infiltration of dilute water will be accelerated by the drawdown towards the open tunnels. This effect is considered to be negligible for the long-term evolution of salinity after closure of the repository and reinstatement of natural hydraulic conditions.

The initial state of groundwater compositions for the regional-scale model at 10,000 years ago, i.e. at the end of the last glaciation and before Littorina sea ingress, is as shown in Figure 1(left). It is composed of 'Deep Saline' water at depth overlain by a mixture of 'Deep Saline', 'Old (Altered) Meteoric' and 'Glacial Melt' reference waters (SKB 2011, p 341). The initial state assigned for matrix porewater compositions is shown in Figure 1(right) with the added feature, as discussed in the previous section, that diffusive exchange for 1000 years has been superimposed on the profile of reference water fractions as shown.

Hydrodynamic mixing of the reference waters and evolution of groundwater compositions are modelled to 10,000 years in the future in the ECPM (equivalent continuous porous medium) regional-scale model. Therefore hydrochemical evolution of the groundwater system is primarily modelled at regional scale as fractions of reference waters. The ECPM is a porous-medium representation of the DFN (discrete fracture network) (SKB 2011, p 340; Joyce et al., 2009). The resulting modelled compositions are used to set groundwater salinities at various future times at nodes in the site-scale and repository-scale DFN models. Regional model outputs are also used to set time-dependent groundwater compositions at the boundaries of the DFN models.

Details of how SKB have used the ECPM model in the ConnectFlow code to simulate the future evolution of salinity are given in documentation for SR-Can and SDM-Site (Hartley et al. 2006; Follin et al. 2007; Follin 2008). SKB have upscaled from a DFN model of transmissive fractures, calibrated with PFL test data, to the ECPM at site scale. Both the site-scale and regional-scale models have deterministic representations of the hydraulic conductor domains (HCDs) which account for most of the large scale groundwater movement and solute transport.

SKB has tested and calibrated the regional-scale model by forward modelling of groundwater mixing, i.e. salinity evolution, from the end of glaciation at 10,000 y ago through to the present day. The forward model is sensitive to the assumed initial conditions and boundary conditions for groundwater and infiltration compositions respectively, as well as to the hydrodynamics of infiltration.

An additional factor influencing the model of salinity evolution is how diffusive exchange with solutes in pore waters in the rock matrix is handled. Diffusive exchange of solutes between fracture waters and pore waters in the rock matrix is simulated in SKB's transport model with an analytical calculation of 1D diffusion from a linear source (infinite parallel equidistant constant-aperture planar fractures) into an infinite matrix (Joyce et al. 2009, p163; Follin et al. 2007). An alternative approach to modelling diffusive exchange, although it is not clear whether this has been implemented in SR-Site, is to assume a matrix of finite thickness. In the latter approach, it is likely that diffusive exchange will be at equilibrium and matrix diffusion will be rather less effective as a retardation mechanism.

Evidence that matrix diffusion will be a significant process in the future evolution of salinity and attenuation of dilute water penetration comes from considering how present-day pore water compositions reflect diffusive exchange in the past. These data have been interpreted in terms of diffusion being effective for several 10s of cm into the matrix, and as evidence that pore waters were dilute prior to the start of Pleistocene glaciations (Waber et al. 2008, p63 and Fig 7-4). Pore waters in the footwall rock FFM01 domain at repository depth are more saline than pore waters in the more fractured hanging wall rock domain which is interpreted to have exchanged with less saline groundwaters probably of glacial origin. Much older pre-glacial groundwaters with a component of meteoric water are inferred from pore water compositions to have circulated in the footwall domain and to have exchanged with the pore waters (Waber et al. 2009, Fig 7-4, p 62).

The regional-scale model simulates how the proportion of meteoric reference water in the system will increase through time, with groundwaters near to the base in parts of the model at 1200 m depth being forecast to have around 90% meteoric component already at 7000 years into the future. Vertical slices through the modelled water compositions at regional scale show that the penetration of dilute water is greatest along the sub-horizontal fracture zones such as A2, and less along the sub-vertical fracture zones such as ENE0060 (Figure 2). The upper cross-section in Figure 2 shows the modelled fractions of the meteoric reference water at the present-day, the model having started at 10,000 y ago with the initial state of reference water fractions as described above in Section 2.1.2. The much lower proportions of meteoric water in the target volume at and below repository depth (see Figure 2) reflect the impact of lower hydraulic conductivity for the footwall rock unit (domain FFM01).

The resulting changes of salinity at repository depth (470 ± 20 m depth) are shown as statistical distributions in box-and-whisker plots for 4 time steps: present day, and 1000, 3000 and 7000 years into the future (SKB 2011, Figure 3, p 358). At the latter time step, 25% of groundwater in the repository volume is modelled to have <3 g/L TDS.

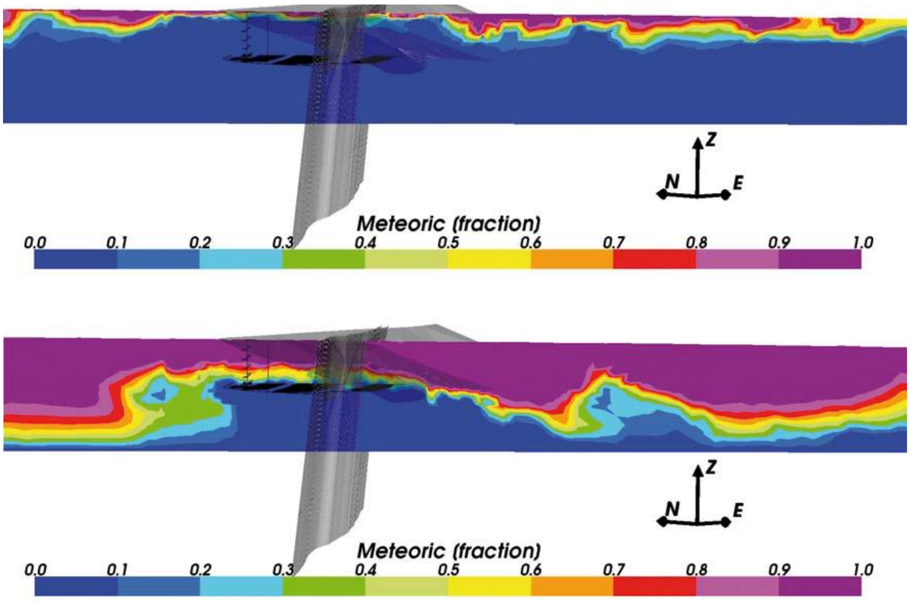

Figure 2: Vertical sections (NW-SE, depth 1200 m) showing proportions of altered meteoric reference water modelled by the ECPM regional-scale model, at present-day (upper) and 7000 years into the future (lower). Gently-dipping deformation zone A2 is shown as a grey plane emerging from the top of the section just left of centre; steeply-dipping deformation zone ENE0060 is shown as a grey plane emerging from the bottom of the model [Figure 10-26 in SKB 2011, p 343; see also Figure 6-4 in Joyce et al. 2010, p 83]

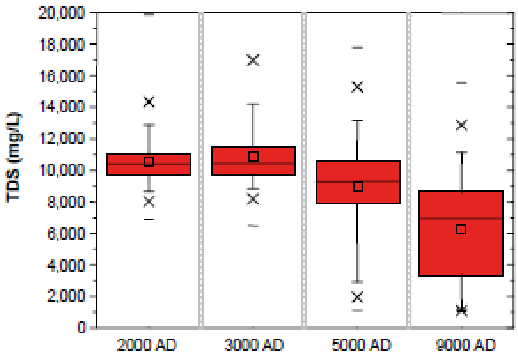

Figure 3: Box-and-whisker plots showing statistical distribution (median, 25th and 75th percentiles, max and min) of TDS concentrations at repository depth in multiple runs of the ECPM regional-scale model. [Figure 10-39 in SKB 2011, p 358]

There are no comparable cross-sections or box-and-whisker plots showing how the advancing ‘front’ of meteoric water will progressively replace brackish and saline fracture waters during the extended temperate period to 60,000 years in the future. SKB summarise results of salinity evolution modelling of the extended temperate climate in Table F-3 (Joyce et al. 2010, p 174). Whereas 42 deposition hole positions would receive water diluted to 5% of the original salinity after 10,000 years, the results indicate that 166 positions would receive similarly diluted water after 60,000 years. The only illustration of these results for the extended temperate period is a cumulative distribution plot of the time for dilute water to reach deposition hole positions, produced by the site-scale DFN model (Figure 4). The modelled F (transport resistance) values for the pathways to the affected deposition hole positions suggest that the efficacy of diffusive exchange with matrix is only one of several factors in controlling which pathways and which deposition hole positions are at risk (Joyce et al. 2010, p 174). Presumably the way that DFN fractures connect with the deformation zone pathways is also an important factor; this is supported by SKB's statement that the affected deposition hole positions tend to be close to areas of high DZ intensity.

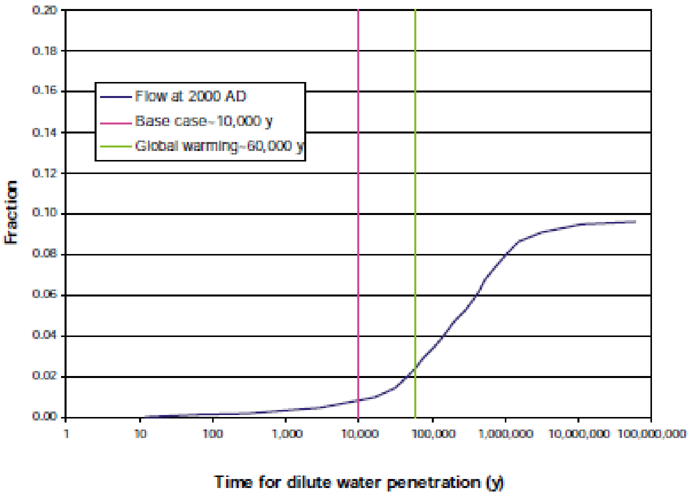

Figure 4: Cumulative proportion of all deposition hole positions receiving dilute water under temperate climate conditions extending for an unlimited timescale. [Figure 10-32 in SKB 2011, p 348; Figure F-8 in Joyce et al. 2010, p 175].

One approach to evaluating the model for regional-scale groundwater flow and salinity evolution is to test the consistency between the modelled distribution of salinity, in terms of TDS, Cl$^-$ or other suitable compositional parameters, and measured concentrations.

Consistency testing and model calibration is done by comparing modelled compositions along a borehole depth profile with measured compositions of water samples. Data and illustrated depth profiles for making such comparisons are not reported in the SR-Site Main Report, although they are reported in the Site Description Report (SDM-Site) and previous modelling reports (see below). SKB states that 'a comprehensive uncertainty analysis with focus on hydraulic parameter heterogeneity within the target volume was performed and the results demonstrate that model calibration against hydrochemical data is sensitive to parameter heterogeneity in the bedrock hydrogeological properties, which is expected in a sparsely fractured rock mass' (SKB 2011, p 135).

A profile for borehole KFM01D is shown in Appendix C of Joyce et al. (2010, pp 147-150) for the purpose of illustrating sensitivity to numerical method and parameters for rock matrix diffusion modelling; this shows modest general match between general values of modelled and measured fracture water Cl$^-$, but no coherence between the shape of the modelled profile and the few available measurements.

Comparisons between modelled depth profiles and measured groundwater and pore water compositions are reported in the Site Description report for SDM-Site (SKB 2008a, Figures 8-46 to 8-50 & 8-68, pp 275-280 & 293) with depth profiles for fracture waters in footwall boreholes (KFM 01A,B,C,D, 02A, 04A, 05A, 06A,B,C, 07A,B, 08A,B,C, 09B) and hanging wall boreholes (KFM 02A & 03A,B) and for pore waters in KFM 01D and KFM 06A (both footwall). In this case more hydrochemical parameters are plotted for fracture waters: Na^+, Ca^{2+}, Mg^{2+}, SO_4^{2-} and Br/Cl, in addition to salinity, Cl^- and stable isotope ratio. Figure 5 shows the modelled salinity profiles in comparison with measurements. From these consistency comparisons for SDM-Site, SKB state that the modelling has improved over preliminary modelling in predicting higher fracture water salinity in the footwall domain than in the hanging wall domain. It also states that simulated pore water profiles of Cl^-, which show higher values than measured below about -400 m, are 'not perfect' (SKB 2005, Figure 8-50). Modelled stable isotope ratios are much lower than measured (SKB 2005, Figure 8-48).

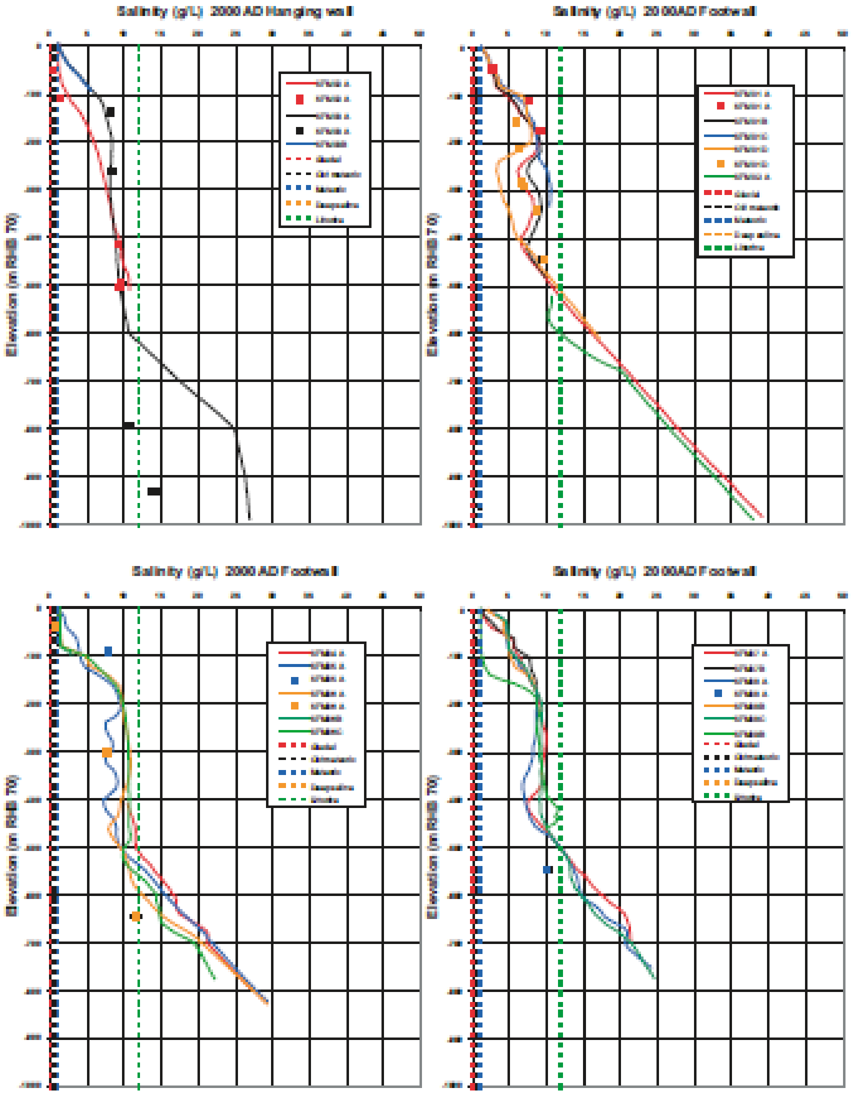

Figure 5: Comparison between regional-scale model simulation of salinities and measured fracture groundwater salinities for boreholes in footwall and hanging wall fracture domains at Forsmark. [Figure 8-46 in SKB 2008a, p 276]

Model calibration of the ECPM is described in Follin et al. (2007) and Follin (2008, Section 7). Simulated hydrodynamic mixing of reference waters in depth profiles corresponding to borehole locations are compared with measured hydrochemical and stable isotope data (Follin 2008, Figures 7-2 to 7-8, pp 100-105). This is done for both fracture waters and pore waters and the results are said to be in 'reasonable agreement'. Sensitivity of the modelled hydrochemical depth profiles to HCD properties, HRD parameters, solute transport parameters including kinematic porosity and flow-wetted surface area, and initial conditions has been investigated (Follin et al. 2007). SKB's conclusion is that, accepting that physical hydrogeological parameters offer the more sensitive calibration, the remaining major sensitivity for salinity evolution is the choice of initial state compositions, particularly for pore waters at 10,000 y ago. SKB has assumed that late Pleistocene/Holocene glacial melt water had not diffused into pore waters to any significant extent, thus leaving the initial condition for pore waters as a mixture between deep saline water and 'old' meteoric/glacial water. Overall, the conclusions regarding calibration are: (a) the assumed initial state distribution of pore water compositions is confirmed, (b) HCD properties are adjusted according to calibration with hydraulic data, (c) vertical hydraulic conductivity of the HRD is increased as also is anisotropy in the DFN, and (d) kinematic porosity of HRD is increased by x10 (Follin et al. 2007, p181). The latter two adjustments would slow the penetration of dilute water.

For the site-scale model, a mixture of flow concepts is used, i.e. continuous porous medium (CPM) and discrete fracture network (DFN), and these are coupled by being embedded so that continuity of pressure and mass flux is ensured (SKB 2011, p 339). Steady-state pressure solutions are derived for time slices, with no advective transport and variation of salinity and no matrix diffusion (unlike what is done for the regional-scale model).

Deformation zones (DZs) are the major pathways by which dilute water moves downwards are they are modelled deterministically in the flow models at all scales. The model parameterisations assume, based on measurements, that maximum transmissivities of the DZs decrease exponentially with depth (see Figure 4-16 in SKB 2011, p 126). Measured transmissivities in many cases are orders of magnitude less than these maxima, so it seems that the parameterisation of hydraulic conductivity in the regional-scale model is pessimistic with respect to dilute water movement. Another aspect of parameterisation of the hydrogeological models is that there are no transmissivity data available below about 460 m, and only about 12 measurements below 400 m, for fractures in fracture domain FFM01, i.e. the target volume (see Figure 4-16 in SKB 2011, p 126). This means that there is a paucity of measurements to calibrate the DFN model for the target volume. It also means that there are no or few transmissivity data to validate the statement that the repository volume is characterised by 'relatively few open fractures' (p 130). SKB comments that confidence is high in the hydrogeological model of the bedrock and that there are greater uncertainties in the properties of the DZs.

Transport properties of flow pathways through the rock influence salinity evolution in fracture waters because these properties control the extent of diffusive exchange of solutes between fracture and rock matrix. Pore waters in rock matrix at Forsmark have been found to have lower salinities than present-day fracture waters, so the overall effect is to reduce the salinity of flowing groundwater. However this effect will be reversed in the future as dilute meteoric water infiltrates. Then diffusive exchange with pore waters will tend to attenuate the advance of dilute groundwaters towards repository depth.

Transport resistance ('F' factor) has been modelled for bedrock conditions at Forsmark and is reported to be around 10^6 years per metre for typical flow paths on a 100 metre scale in the FFM01 domain at >400 m depth, i.e. at repository depth

(SKB 2011, p 137). Major deformation zones such as gently-dipping A2 are shown to have F values that are lower by several orders of magnitude, so FFM01 rock surrounding deposition holes would contribute the greater part of retardation of released radionuclides and similarly provide an important attenuation of dilute water.

Numerical DFN simulations of flow and transport to repository depth also show that <4% of the DFN realisations for domain FFM01 at >400 m depth are connected such that dilute water would be transported through them to deposition hole positions.

Hydraulic gradients that have been inferred from field measurements of natural groundwater flow are higher than modelled hydraulic gradients and generally exceed the gradient suggested by topography by ‘orders of magnitude’ (SKB 2011, p 128). Tracer dilution tests also suggest larger flow rates than are ‘reasonable’ (SKB 2011, p 128).

2.1.4. Modelling of dilute water infiltration and salinity evolution through a future glacial period

The penetration of dilute water associated with a future glacial period in the reference evolution is modelled in a very similar way to that above for dilute water during the temperate period. Hydrogeological boundary conditions for the repository-scale and site-scale models are taken from Vidstrand et al. (2010) in which melt water penetration was simulated with the model code DarcyTools plus an analytical expression for matrix diffusion.

Unlike the modelling of salinity through the temperate climate period, the model of salinity evolution during a glacial climate period does not simulate mixing between reference waters. Rather, it has an initial condition expressed in terms simply of salinity, defined by a mixture of deep saline reference water and meteoric water. Addition of glacial melt water results in a progressive dilution of this initial water salinity.

Glacial melt water, assumed to have zero salinity, recharges thorough pathways that originate close to the surface. The only process that affects salinity during flow through the fracture network is diffusive exchange with pore waters in the rock matrix. Salinity of the pore water at the start of the modelled period is assumed to be at equilibrium with adjacent fracture waters prior to the episode of glacial melt water ingress. In the illustrative model runs, the salinity of fracture waters prior to melt water ingress is assumed to be 3 g/L TDS. The evolution of salinity is illustrated in Figure 6. The duration of temperate conditions and meteoric water inflow that has been modelled to give the top cross-section of salinity in Figure 6 is not stated. The regional-scale hydrogeological model also calculates corresponding Darcy fluxes. The model results show a zone in front of the edge of the advancing/retreating ice sheet, for the case without permafrost under the ice sheet, where groundwater flows are directed quite strongly downwards (see Figure 10-129 in SKB 2011, p 494).

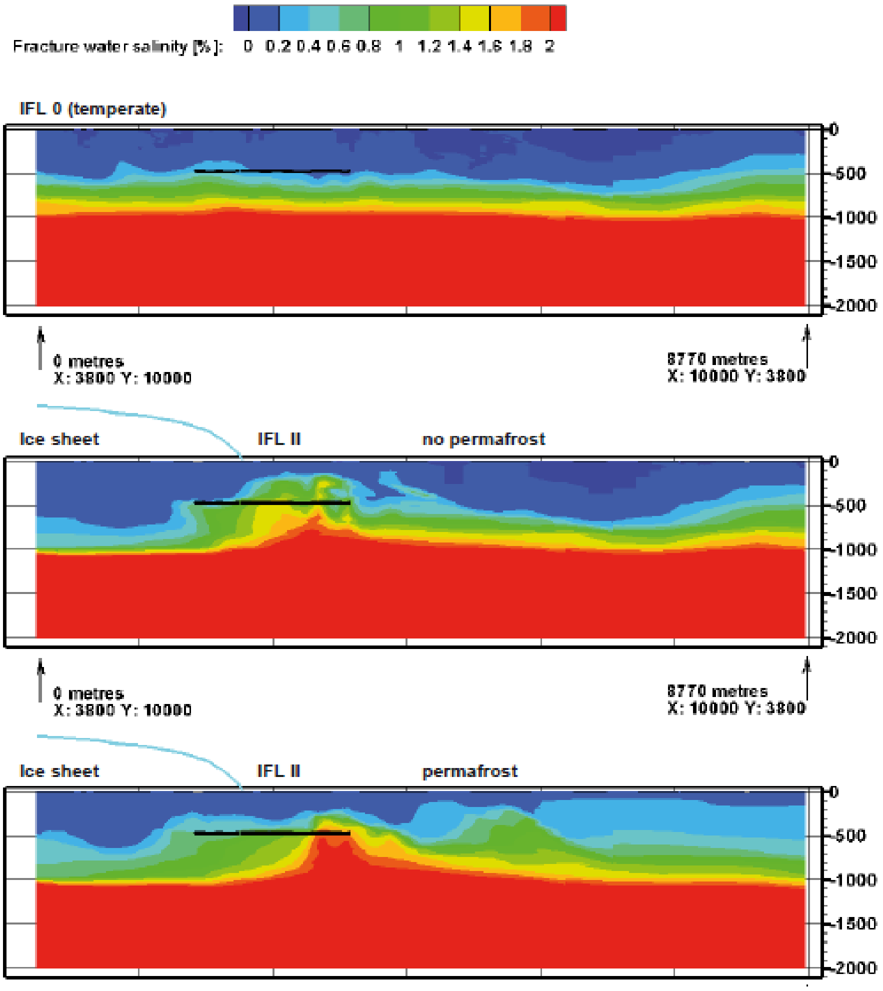

Figure 6: Evolution of salinity through temperate conditions just prior to the advance of ice over the site (top) and glacial conditions (middle - without permafrost in front of ice sheet, bottom – with permafrost). [Figure 10-130 in SKB 2011, p 495]. [Note: it is unclear what duration of temperate conditions is illustrated in the top section].

Temporal changes of Darcy flux and salinity at repository depth for various positions of an ice sheet in relation to the repository footprint are shown in Figures 10-132 to 10-135 in SKB (2011, pp 497-499). They show salinity reduction to <10% of initial salinity transiently at the start and end of a glaciation of about 19,000 years duration, i.e. at times when the front of an advancing or retreating ice sheet is close to the repository location (Figure 10-134). Dilute water penetration is greater for a slower average speed of a retreating ice sheet (Figure 10-135).

The DarcyTools model used in Vidstrand et al. (2010) is not capable of the level of discretisation that is needed to model penetration of dilute water at the scale of deposition holes. So boundary conditions from this model have been used with the ConnectFlow DFN model as described in Joyce et al. (2010, pp 116-127) to simulate the penetration of glacial melt water at repository scale. The only process that mitigates penetration of dilute melt water (zero salinity) is out-diffusion into fracture waters of salts from the matrix pore waters (Joyce et al. 2010, Appendix F).

SKB's base case model of glacial melt water infiltration assumes that the maximum duration that an advancing ice sheet in the vicinity of the repository footprint will be enhancing groundwater movement to deposition holes will be 100 years. SKB's model indicates that, in those conditions, 2% of deposition holes (i.e. 147 holes) would experience water that has been diluted below 10% of the original salinity, i.e. to less than 0.3 g/L TDS (Figure 7; Table F-4 in Joyce et al. 2010, p 179). If the ice sheet were to halt for only 20 years, the model estimates that 77 deposition holes would be affected. A variant DFN model with extended spatial variability gives slightly lower numbers of affected deposition holes: 99 and 44 respectively (Joyce et al. 2010, p 178).

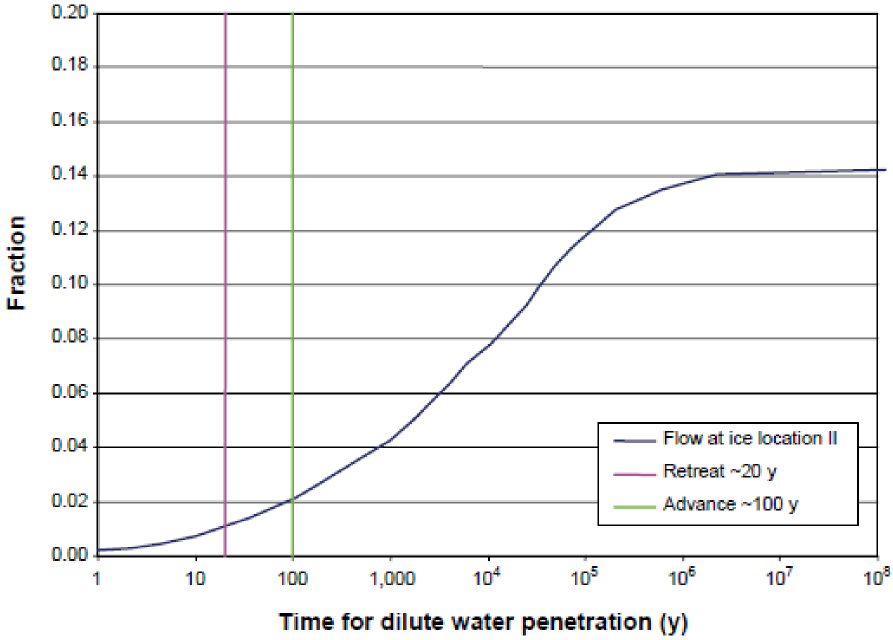

Figure 7: Fraction of all deposition hole positions receiving water diluted to 10% of initial salinity during the glacial climate period, as a function of the time for which an advancing ice front would be stationary close to the repository footprint without permafrost at the base of the ice sheet. [Figure 10-139 in SKB 2011, TR-11-01, p 503 & Figure F-10 in Joyce et al. 2010, p 176].

The model also indicates that the period of total ice sheet cover of the repository location would have to continue for 100,000 years to get a similar proportion of deposition holes being affected (Figure 8).

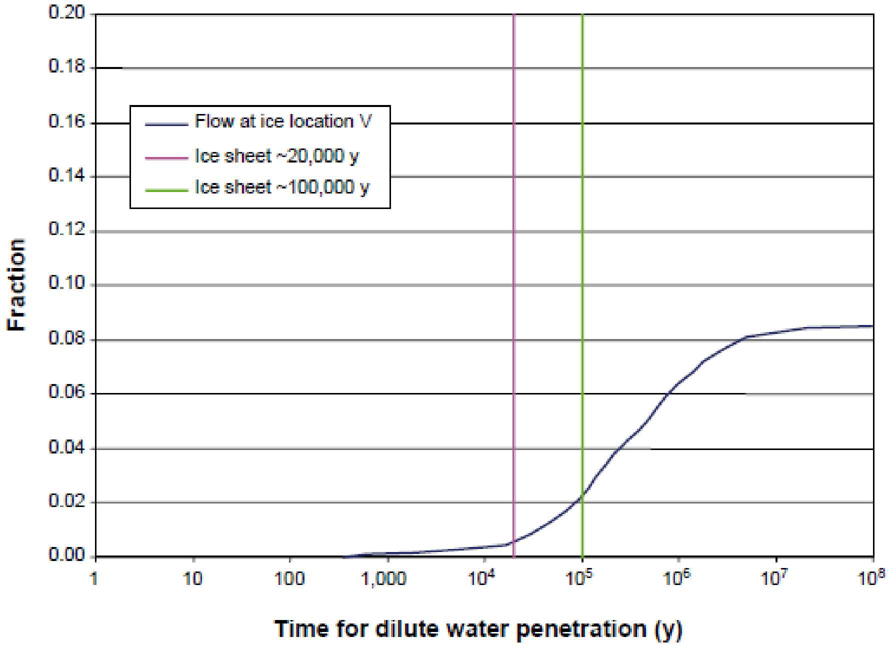

Figure 8: Fraction of all deposition hole positions receiving water diluted to 10% of initial salinity during the glacial climate period, as a function of the time for which the centre of the ice sheet would be located above the repository footprint. [Figure 10-140 in SKB 2011, p 503 & Figure F-12 in Joyce et al. 2010, p 177].

Thus the hydraulic conditions and duration of advancing and retreating ice sheet conditions that would cause incomplete ice sheet cover would seem to be critical factors to be considered with respect to the probability of dilute water reaching deposition holes. Orientation of ice sheet advance and retreat, and existence of permafrost ahead of the ice front that would affect hydraulic behaviour of melt water are other factors that have been considered in SKB’s conceptualisation and scoping model, but it is concluded that none of the variants give significantly different results from the base case (SKB 2011, pp 504-508 & 510).

The reference glacial cycle evolution of the Forsmark site out to 120,000 years in the future has two major ice sheet advances, one at about 60,000 years after present and a second at about 100,000 years after present (SKB 2011, Fig 10-107, p 450). The former is shorter than the latter which has a duration of about 20,000 years. SKB infers that no deposition holes would be exposed to dilute water during the first, shorter, glaciation.

SKB also infers, cautiously, that deposition holes with the highest groundwater flow rates could be exposed to dilute water for 30,000 years of the 120,000 years period, i.e. 25% of the time (SKB 2011, pp 528-529). From this, and using the base case hydrogeological model which has a semi-correlated DFN and having complied with the proposed acceptance criteria for deposition hole positioning, SKB forecasts that one deposition hole will suffer buffer erosion to the point of reaching advective conditions for the last 30,000 years of the 120,000 years reference glacial cycle. Similarly, it is forecast that 23 deposition holes could reach advective conditions in 1 million years. This modelled outcome for advective conditions is less adverse than the 2% of 6000 deposition holes being exposed to dilute water that is assumed in the safety analysis (SKB 2011, p 529).

Evolution of groundwater composition during periglacial conditions is mainly concerned with the potential effects of increasing salinity of residual groundwater during freeze-out of salts when permafrost forms (SKB 2011, pp 512-513). This process has been modelled generically by Vidstrand et al. (2006) and with site-specific parameters (but neglecting diffusive exchange of salts between fracture water and pore water) by Hartikainen et al. (2010). In brief, the outcome of these simulations is that no more than a small increase of salinity should be expected at repository depth for the most extreme permafrost conditions. Subsequent thaw of permafrost would possibly release water into the system that is more dilute than deeper unfrozen groundwater. Brackish salinity of 2-4 g/L during this stage of evolution has been modelled for repository depth (SKB 2011, Fig 10-148, p 513; Salas et al. 2010).

Among the uncertainties that SKB has identified in the models dealing with groundwater flow and compositions during periglacial and glacial conditions are (SKB 2011, pp 509-510):

- Palaeohydrogeological evidence of groundwater evolution considered in SDM-Site and modelling done by Vidstrand et al. (2010) suggest that transient changes in advective flow rather than matrix diffusion have the greater effect on fracture water salinity. This conclusion differs from the conceptualisation of dilute water penetration to repository depth used above, which is therefore inferred by SKB to be a pessimistic simplification for long-term evolution through a glacial cycle.

- In the site-scale DFN model, a number of particles recharge at the upstream boundary of the model domain, suggesting that the model domain is too short to give a fully undisturbed view of all recharge locations. It is concluded that the present-day topographic water divides, which play an important role for the recharge and discharge during temperate conditions, are significantly diminished in significance during glacial conditions.

- The transfer of boundary conditions for glacial conditions from the super-regional model to these smaller-scale models implemented in a different numerical flow code introduces uncertainties.

- The assessment of penetration of dilute water should be considered an approximate quantification. The same uncertainties as for the corresponding analyses performed for temperate conditions apply. Specifically, steady-state flow fields are used, and no mixing or water-rock interactions are considered.

- The use of scaling factors for comparing Darcy flux at different times during glaciation and deglaciation is a simplification of the development of climate regimes in the Climate report (SKB 2010c), and hence implies an additional uncertainty. For the safety analysis, the hydrogeological model of glaciation has permafrost in front of an advancing ice sheet margin and submerged ground conditions in front of a retreating ice sheet. SKB suggests that climate stages with permafrost alone and submerged conditions alone also need to be included in the quantitative assessment.

2.1.5. Modelling of groundwater flow and dilution at deposition hole positions

The coarse discretisation of the regional-scale model does not allow groundwater composition evolution to be simulated in sufficient detail for specific deposition holes. So an alternative, simplified approach has been used for repository-scale modelling in SR-Site (SKB 2011, p 347).

SKB has constructed the discrete fracture network (DFN) representation of transmissive fractures, i.e. the hydrogeological DFN, on the basis of the geological structural model and DFN plus information from geophysical logging and hydrogeological testing of identified structures. The hydrogeological DFN at repository tunnel and deposition hole scale is a stochastic representation of fractures and transmissivity distribution in the ‘intact’ bedrock in which deposition tunnels and holes will be located. Connected pathways for dilute water to move from near the surface towards repository location are modelled in terms of percolating fracture networks, represented stochastically, plus the major faults and fracture zones, represented deterministically.

At the repository scale, three blocks are modelled separately for reasons of practicality. Bedrock surrounding the tunnels plus ramps, shafts etc. is modelled as a DFN but some features are embedded as porous medium elements, i.e. main tunnels, deposition tunnels and deposition holes. Steady-state pressure solutions are derived with fixed salinity field for time slices at which the boundary pressures and water densities have been calculated for the regional-scale model with the ConnectFlow code. As for the site-scale model, advective transport of salinity and matrix diffusion are not explicit in the numerical model but rather are represented by an analytical solution (SKB 2011, pp 338-339).

Particle tracking produces cumulative advective travel times and flow-related transport resistances for released particles, and also Darcy fluxes and equivalent flow rates, Q_{eq}, at deposition hole positions for groundwater in the DFN. These flow rates are used as input to the buffer erosion-corrosion analyses. Reverse particle tracking is used, i.e. three particles are released from each deposition hole position – one for each of the radionuclide release paths (Q1: fracture intersecting deposition hole; Q2: through the EDZ; Q3: through the backfilled tunnel and a fracture intersecting the deposition tunnel; see Fig 13-12 in SKB 2011). Each of these particle paths are extended into the site-scale model at the exit location on the edge of the repository-scale model.

The assessment of the potential for penetration of dilute water to each deposition hole location at repository depth has been based on these groundwater recharge paths from the repository-scale model and an analytical solution for solute transport using the flow-related transport properties (SKB 2011, pp 339-340; Joyce et al. 2009, Appendix F).

Water with zero salinity is infiltrated at the top surface of the repository-scale DFN model (SKB 2011, p 347), which is a pessimistic assumption in comparison with the regional-scale model which has the altered meteoric reference water infiltrating through the top boundary.

The proportion of deposition hole positions that would never experience dilute water penetration, according to the repository-scale DFN modelling, because they are not intersected by a DFN fracture, is illustrated in Figure 9. Just over 70% of deposition hole positions have a vanishingly low Darcy flux, i.e. zero advection, for the Q1 pathway. If the full perimeter criteria (FPC) or extended full perimeter criteria (EFPC) are applied to reject vulnerable deposition hole positions, the proportion of positions that have zero advection rises slightly to just under 80% if both FPC and EFPC are applied.

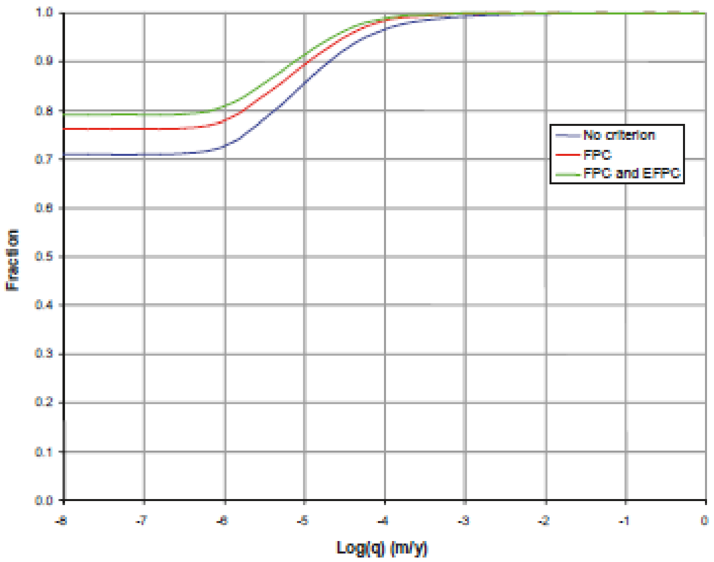

Figure 9: Cumulative distribution plot of Darcy flux (q) for the Q1 path for all deposition hole positions for present-day groundwater conditions, with/without the deposition hole rejection criteria (FPC & EFPC) being applied. [Figure 10-30 in SKB 2011, p 346; also see Figure 6-15 in Joyce et al. 2010, p 92]

Only those particle tracking flow paths in the DFN model for the present day that connect deposition holes with recharge points ‘close’ to the surface are selected for salinity evolution modelling (SKB 2011, pp 347-348). Initial salinity distribution in fracture waters is as previously described, and initial matrix water salinity is assumed to be in equilibrium with adjacent fracture water. Meteoric (zero salinity, see above) or glacial water is recharged along each of the flow paths. Salinity of the recharging water is increased only by diffusive exchange with matrix water. For each deposition hole location, the time taken for salinity to fall to less than 10% of the initial salinity (i.e. 10% of ~10 g/L, or 1 g/L) at that location in the DFN is calculated by the model.

The results indicate that just under 1% of all deposition holes (noting that anyway only 20-30% of deposition holes will experience advective flow, as shown in Figure 7) would be thus affected after 10,000 y, assuming that the flow conditions continued as they are at present (Figure 4). For the variant climate scenario whereby global warming would prolong the temperate period, the model suggests that slightly more than 2% of deposition holes would be affected by dilution to <10% of initial salinity after 60,000 y (Figure 4). In its assessment of identified uncertainties in this modelled forecast, SKB state that it “should be considered an approximate quantification”. The main reasons for that are: (a) the present-day flow conditions are used in the DFN model, and (b) no mixing or water-rock reactions are considered, thus discounting processes that would increase salinity. It states that these “rough estimates” are appropriate for use in analyses of buffer erosion and corrosion because they are likely pessimistic, supported by the site descriptive model that indicates that dilute groundwaters have not penetrated to that depth in the past.

The thermo-hydro-mechanical (THM) effects of glaciation on the reactivation and transmissivity of fractures through a glacial cycle has been modelled by Hökmark et al. (2010), SKB (2011, pp 459-460). The potential increase are said to be "very moderate" and are thus considered to be negligible in the safety analysis.

2.1.6. Evolution of groundwater compositions due to water-rock reactions

SKB emphasises the 'key importance' of reactions with fracture minerals and bedrock for groundwater compositions especially with regard to hydrochemical evolution following infiltration of dilute and oxidised water (SKB 2011, p 133). Calcite is widespread, in the surficial glacial sediments and as a secondary mineral in fractures throughout the bedrock, and is the main buffer of pH and related hydrochemical parameters, bicarbonate, P_{CO2}, and Ca^{2+}. The other set of reactions that are of prominent interest are ones involving iron oxide and iron sulphide minerals and thus buffer redox conditions and attenuate any dissolved oxygen that might enter the groundwater system in the future, for example in glacial melt water. Amorphous iron oxyhydroxide mineral occurs in transmissive fractures and fracture zones, such as A2, at shallow depths. This is interpreted as evidence that past oxygen infiltration has been attenuated by reaction with reducing minerals such as iron sulphides. Observed reducing conditions in groundwaters are evidence that this buffer capacity is maintained and will continue to influence groundwater compositions in the future, for example with mineral sulphide being oxidised to sulphate and iron being dissolved.

The hydrogeochemical evolution of groundwater compositions over time is modelled for SR-Site using the regional-scale hydrogeological model (using the ConnectFlow code) to generate spatial distributions of mixing proportions between the various reference waters at various times to 7000 years in the future. These proportions, for various points in the site volume, are input to the PHREEQC code for mixing and water-rock reaction (Salas et al. 2010).

The reactions that are modelled are equilibria with calcite, quartz, hydroxyapatite, and either Fe(III)-oxyhydroxide or amorphous Fe(II)-sulphide (SKB 2011, p 355). Ion exchange is not simulated. None of these reactions are taken into account directly in the DFN-based model for dilute water flow towards deposition holes.

2.1.7. Assessments of confidence and uncertainties

The forecasting of salinity evolution at repository depth and of the probabilities of dilute water penetration to deposition holes contains a number of modelling elements where degrees of confidence and the potential magnitudes of uncertainties should be assessed. These are:

- Reference water compositions;
- Initial state for groundwater compositions at 10,000 years ago;
- Regional-scale ECPM modelling of salinity evolution in the temperate and glacial periods;
- Site-scale and repository-scale DFN modelling of dilute water entering deposition holes;

- Hydrogeochemical modelling of water-rock reactions affecting dilute water compositions.

Confidence and sources of uncertainties in the assigned compositions of reference waters have been studied in Gimeno et al. (2008). SKB comment that there are many potential uncertainties in the assigned compositions (SKB 2008b). Single values cannot represent the likely temporal and spatial variabilities of the various components that have mixed and constituted present-day groundwaters. SKB state that 'the uncertainties are bounded to the extent possible regarding postglacial and present day scenarios' (SKB 2008b, p 36). There are also similar uncertainties in their representation of mixing components in the future.

The deep saline and altered meteoric reference waters correspond to actual measured groundwater compositions. The Littorina and glacial reference waters represent old waters and therefore cannot be measured, however the assigned compositions are justified. The 'old' meteoric reference water has been introduced into the modelling at a late stage as a way of explaining the variations of salinities below repository depth without having glacial water penetrate to unreasonable depths (the stable isotope compositions are evidence against that). SKB has assessed the impacts of uncertainties in reference water compositions mainly in terms of the M3 PCA modelling which 'disaggregates' measured groundwater compositions into proportions of the reference waters. SKB has also shown that the mixing model with 4 chemical and isotopically distinct reference waters plus the additional isotopically-distinct old meteoric reference water is consistent with the variation of actual groundwater samples in the sequence of presumed temporal evolution (Gimeno et al. 2008, p 61). This adds further to confidence in both the palaeohydrogeology and the selection of reference waters to describe mixing.

Monte Carlo computations have been used to find the reference water compositions (for 4 reference waters, excluding 'old meteoric' water) that, combined with values for mixing proportions, give the minimal residuals when the complete set of hydrochemical data are analysed by the M3 PCA method. This study has contributed a large degree of confidence to the use of the M3 method and the assigned reference water compositions. For some of the reference waters, it has shown that the mixing proportions are rather insensitive to the assigned compositions over wide ranges (Gimeno et al. 2008). SKB reports that the two reference waters for which the Monte Carlo calculations have pointed to discrepancies with the prior 'hydrochemically-based' compositions are (i) the stable isotopic composition of the glacial reference water, and (ii) the Cl^- concentration of the altered meteoric reference water (Gimeno et al. 2008, p 46). Referring to the second issue, it states that selection of the altered meteoric reference water is 'a critical issue in the dilution scenario for the temperate period' and that 'all elements except Ca^{2+} are well constrained by the Monte Carlo method (Gimeno et al. 2008, p 49).

The assignment of proportions of reference waters in the depth profile of groundwater compositions that are used as the initial state, at 10,000 years ago, for salinity evolution modelling has been supported by M3 PCA analyses of brackish groundwater samples from intermediate depths at Forsmark (Gimeno et al. 2008, p 50), as well as by expert judgement. The variability of M3 PCA analyses which is due to using the rather arbitrary reference water 'old meteoric-glacial' has also been investigated and found, as expected, to only affect the relative proportions altered meteoric and glacial or old meteoric-glacial reference waters. Two further data-based approaches to deducing the most likely pre-Littorina compositions, at 10,000 years ago, have been used to add weight to the initial state reference waters and mixing proportions. Overall, SKB's conclusion is that the most likely Cl^- content of initial state waters down to repository depth is 3500-4500 mg/L (Gimeno et al. 2008, p 58).

The role of salinity and density differences as the cause and control of Littorina intrusion into the initial state mixture has also been studied (Gimeno et al. 2008, p 60). This more or less confirms the theoretical expectation that Littorina would have penetrated deeper into rock volumes in which the salinity and thus density of pre-Littorina groundwater was lower, i.e. giving a larger density differential and therefore allowing gravity to promote Littorina infiltration. However SKB conclude that other hydrodynamic factors may also have an additional role. The importance of this for present purposes is that it supports the concept that future dilute water movement towards the repository volume would be subject to similar variable density effects on groundwater movements.

An overall conceptual model for the palaeohydrogeological temporal evolution of groundwater compositions is consistent with most of the groundwater compositions at the Swedish and Finnish sites on either side of the Gulf of Bothnia and also with the theoretical conceptual hydrology of the system. SKB concludes that this strengthens the confidence in the proposed mixing history. Moreover the absence of significant amounts of the Littorina component in at least parts of the FFM01 fracture domain, in contrast to its widespread presence in deformation zones and in the more fractured domains, reinforces the interpretation that the target volume rock has a low frequency and low transmissivity of fracturing that makes it resistant to gravity-driven intrusion under normal gradients (Gimeno et al. 2008, p 134).

Confidence and remaining uncertainties in the regional-scale ECPM modelling of future salinity evolution have been addressed in Follin et al. (2007, 2008) and in SKB (2008b). In particular, the parameter changes that were implemented to calibrate the palaeohydrogeological ECPM solute transport model against present-day salinity distributions. Both kinematic porosity and flow wetted surface area were increased, the former by about an order of magnitude from an empirical relationship and the latter by up to two orders from the fracture frequency suggested by PFL measurements. In the case of flow wetted surface area, an extremely low value, $<0.01\ m^2/m^3$, for FFM01 rock at <-400 m depth has been increased for 'pragmatic' reasons to $0.15\ m^2/m^3$ (Follin et al. 2000, p 192). This is potentially significant for salinity evolution and penetration of dilute water to deposition holes because the raised value would facilitate greater diffusive exchange and therefore attenuation of dilute water. On the other hand, sensitivity testing of palaeohydrogeological simulations of salinity and Cl^- depth profiles for comparison with observed profiles indicates that the simulations in multiple realisations are rather stable to changes in structural-hydraulic properties (Follin et al., 2008, p 125).

In the 'confidence assessment' report for SDM-Site, SKB state that 'the understanding of processes occurring during a glaciation is less good and uncertainties exist, especially in relation to buffering against infiltrating dilute groundwater' (SKB 2008b, p 6). Evidently, these uncertainties in glacial processes, especially hydrology, should be superimposed on uncertainties in the hydrogeological and transport properties of the bedrock system.

In considering alternative models or hypotheses, the alternative models that SKB thinks should be propagated to safety assessment include those that consider alternatives in the DFN model for fracture frequency, properties and connectivity

(SKB 2008b, p 6). These features and properties would influence the penetration of dilute water to deposition holes. In particular, fracturing and transport properties of the bedrock surrounding deposition holes are of primary concern. SKB states that ‘the extent of the low permeable volume needs firmer confirmation’ and ‘whether it can be described by a traditional DFN, or whether it is an extreme channelling system’ needs further assessment (SKB 2008b, p 14 & pp 31 & 63). However the issue of uncertainties and alternative concepts for DFN models are outside the scope of this report, although it is evidently one of the factors in the modelling of dilute water penetration to deposition holes. SKB considers that the uncertainties in this issue are much reduced compared with previous model versions. Consistency within larger sets of hydraulic testing data especially for domain FFM01 increases confidence ‘that the rock mass between the transmissive DZs is a very low permeable medium, but the interpretation is uncertain’.

Concerning transport properties that would influence both radionuclide migration and salinity evolution through exchange with pore waters, SKB state that the flow channel frequency in the repository volume may be underestimated, but assert that the overall F factors for typical flow paths should not vary greatly (SKB 2008b, p 40). Uncertainties in the transport properties of the DFN fractures ‘can be bounded’. Overall, however, there is rather little consideration of salinity evolution directly in the Confidence Assessment report for SDM-Site (SKB 2008b), presumably because salinity evolution and dilute water penetration modelling is a safety assessment issue and not a site description issue.

The model for bentonite dispersion and loss from a deposition hole calculates the rate of loss from (a) duration of persistence of groundwater composition with <4 mM charge equivalents of cations, (b) groundwater velocity at the point where a fracture intersects a deposition hole, and (c) fracture aperture (Neretnieks et al. 2009). A mechanical model for buffer loss, which is relatively pessimistic in conceptualising that bentonite swelling would be restricted by friction, is used in the safety analysis. Amongst the arguments for this approach, it is said to allow for temporal and spatial variations in groundwater composition and thus also of buffer porewater compositions (SKB 2011, p 401).

SKB has evaluated the robustness of the safety case to water inflow, buffer erosion and canister corrosion by combining probabilistically the distributions of groundwater flow and salinity from the DFN model with the distributions of dissolved sulphide in groundwaters at deposition hole locations (SKB 2011, pp 532-533).

Probabilistic assessments using the semi-correlated hydrogeological DFN model, implementation of the EFPC criterion for acceptance of deposition hole positions, distribution of sulphide concentrations and pessimistic corrosion geometry, give mean numbers of failed canisters as 0.087 to 0.12 within a million years (SKB 2011, p 533). The robustness towards the maximum likely sulphide concentration and the distribution of flow rates at deposition holes is shown by SKB’s modelling result that only 4 deposition holes would have sufficiently high flow rates that, if inflowing water were dilute enough to breach the safety function and if combined with the maximum of the sulphide concentration range, erosion would lead to buffer loss and advective conditions and corrosion would lead to canister failure within a million years. Doing a similar probabilistic assessment but using the hydro DFN variants with uncorrelated and correlated models for transmissivities versus fracture size, gives averages of 0.65 and 0.57 failed canisters within a million years.

Even if buffer loss and advective water flow directly to canisters is assumed from time zero, the numbers of failed canisters only roughly doubles (SKB 2011, p 533). This indicates that corrosion rates that are constrained by maximum sulphide concentrations and maximum inflow rates are the dominating factor in the timing and number of canister failures. SKB claims that the canister design is robust, even allowing for the remaining uncertainties in buffer performance and resistance to erosion.

Notwithstanding that demonstration of robustness to uncertainties about the buffer erosion process, SKB reports calculations of the sensitivity to amount of buffer loss required for advective conditions to occur and to the assumptions and constraints in the hydrogeological DFN (SKB 2011, Fig 12-3, p 579). For the base case with semi-correlated hydro DFN, 0.6 deposition holes on average would have advective water flow to the canister after 100,000 years rising to 19 deposition holes after 1 million years. In the worst cases of (i) continuous erosion in all deposition holes from time zero, (ii) pessimistic fracture aperture size and thus higher flow rates, and (iii) uncorrelated variant of the hydro DFN, averages of 3.9, 7.5 and 1.2 deposition holes respectively would have advective flow to the canisters, rising to 222, 575 and 279 respectively over a million years. These calculations indicate that the groundwater inflow rates at deposition holes and spatial distribution of fractures, both of which are dependent on the DFN model, are the key factors in rate and location of buffer loss and onset of advective flows to canisters.

These sensitivity calculations with the hydro-DFN model use the base case assumptions and pore water exchange model for distribution of groundwater salinities. In other words, they assume the duration and distribution of dilute water penetration to deposition holes that is output by the base case model. Therefore these calculations do not assess directly any alternative models or assumptions for salinity evolution and dilute water distribution, temporally and spatially. However, sensitivity to groundwater composition has been checked implicitly by one of the ‘worst case’ variants that assumes that erosion would take place throughout the 1 million year assessment timescale rather than through only 25% of it. Under that condition of continuous erosion, the number of deposition holes experiencing advective conditions is calculated to be 3.9 after 100,000 years and 222 after 1 million years as stated above.

It is noted that SKB raise the possibility of revising the design premises such that deposition holes with potential for high Darcy flux should be avoided so as to minimise the chance of piping erosion in the initial period after buffer emplacement. This would be in addition to the FPC/EFPC criteria and also in addition to an existing requirement to limit water entering deposition holes before saturation to 150 m^3 (which anyway is not practicably measureable). Such a measure would, in principle, also lower the modelled rates of canister failures due to chemical erosion of buffer and canister corrosion for the variant scenarios described above. SKB’s tentative suggestion is to reject deposition holes that are intersected by connected transmissive fractures capable of producing groundwater inflows higher than 0.1 L/min (SKB 2011, p 829).

2.1.8. Further work to reduce uncertainties

SKB has accepted that further studies will be needed to reduce the uncertainties discussed above concerning the DFN model for fractures in the target volume. Additional evidence is needed to confirm the validity of the general DFN concept and the key parameters in it such as fracture frequency in the bedrock domain FFM01, and to preclude the possible validity of alternative concepts such that of extreme channelling of flow in the vicinity of deposition holes.

Apart from additional evidence to support the DFN parameterisation, SKB does not discuss further work that might reduce uncertainties in other aspects of the model for salinity evolution and dilute water penetration. Other aspects of the salinity evolution model where there are significant uncertainties are the accessibility of matrix to diffusive exchange, the effective flow-wetted surface, and diffusivity of the matrix.

I assume that SKB would monitor inflows intensively during the construction and operation phase, in conjunction with fracture mapping and implementation of the FPC/EFPC methodology for acceptance. Monitoring the distribution of salinities and comparison with the expected distribution would be an obvious step towards building confidence in the assumptions made in the salinity evolution modelling.

2.2. Motivation of consultant’s assessment

2.2.1. Modelling of long-term salinity evolution

In the normal evolution scenario for the KBS-3 repository, the chemical composition of groundwater at repository depth will change over the long term following repository closure and resaturation of the tunnels and deposition holes.

It will change progressively as the current temperate climate continues due to an increasing and dominant proportion of dilute meteoric water that infiltrates due to land uplift and complete subaerial exposure of the land surface surrounding the repository footprint. Trajectories of downflowing groundwater flow paths and of discharging flow paths may also change as the hydrogeology of the system changes in response to land rise and shoreline recession. The likelihood of global warming means that the temperate climate state may be prolonged substantially beyond the duration envisaged in the normal evolution. Therefore it is very likely that dilute water will infiltrate under temperate conditions for considerably longer than is envisaged by the normal evolution scenario. This probability has been taken into account by a ‘global warming’ variant scenario in SKB’s safety analysis.

A prolonged period of temperate climate and of dilute water infiltration would increase the likelihood of dilute water penetrating to deposition holes and coming into contact with buffer. Theoretical and empirical evidence suggests that compacted bentonite may disperse as a colloid and thus be eroded if the dissolved concentration of cations in groundwater contacting the buffer are below a threshold. Erosion of buffer would eventually lead to a state of de-compaction that would allow water to move advectively towards the canister surface. That would increase the transport of sulphide to the canister and thus increase the rate of copper corrosion.

The significance to SKB’s safety case of this variant scenario for prolonged dilute water infiltration and potential buffer erosion and canister corrosion is that it is potentially the most plausible combination of FEPs (features, events and processes) to exacerbate the canister failure rate and thus lead to relatively early releases of radionuclides, i.e. at times when the radiological inventory has decayed less than would otherwise be the case.

Dilute water intrusion from melt waters during a glacial climate state, which comes relatively early (ca. 30,000 y) in the normal evolution scenario and much later in the global warming variant scenario (ca. 70,000 y), would have a similar impact on groundwater compositions at repository depth. There is evidence that isotopically distinct 'cold-climate waters' penetrated several hundred metres and possibly to repository depth during past ice ages, though it is not known how dilute those groundwaters became. There is substantial uncertainty about the hydrogeological processes under an ice sheet and the potential range of groundwater compositions that might result, more so than the uncertainty about salinity evolution during a prolonged temperate period.

An additional consideration in how groundwater salinity will evolve through these long-term climate changes is the additive effect in groundwater salinity evolution of glacial melt water intrusion following a prolonged period of dilute water infiltration through a temperate climate period. A third climate state, periglacial conditions, will prevail between the temperate and glacial states. This also might have implications for groundwater movements and compositions although the consensus is that permafrost formation will strongly reduce infiltration and make the groundwater system at repository depth more or less stagnant. Although there are many uncertainties in this assumption about periglacial hydrogeology, as there are with sub-glacial hydrogeology, it can be concluded that the greater risks of severe groundwater dilution leading to erosion of buffer in deposition holes occur for temperate and glacial periods of climate and groundwater evolution.

The motivation of this assessment is therefore (a) to review and evaluate SKB's model development and parameterisation for forecasting groundwater salinity evolution at repository depth and dilute water penetration to deposition holes; (b) to consider whether there are viable alternative models and/or parameters that SKB has not considered; (c) to check whether assumptions and simplifications in SKB's modelling and parameterisation are reasonable; and (d) to give an expert judgement on the weight of SKB's modelled evidence and associated arguments that the probability of the buffer's safety function being disrupted by dilute water inflow and chemical erosion is significant in only a small number of deposition holes.

2.2.2. Safety function indicator for buffer erosion

It is appropriate to have a brief explanation of how long-term salinity evolution towards dilute groundwaters in the repository system poses a potential problem for buffer performance and of the origin of the safety function indicator criterion.

The process model and parameters for buffer erosion due to mobilisation of bentonite as a colloidal sol are described in detail in the Buffer, Backfill and Closure Process Report for SR-Site (SKB 2010) and in Neretnieks et al. (2009). Essentially, the colloidal behaviour of flat charged surfaces, i.e. coagulation or sol dispersion, is dependent on the charge equivalent of the interlayer solution. That is expressed as a critical coagulation concentration (CCC) which can be calculated from colloid theory. CCC can be modelled for monovalent cations but is not strictly valid for divalent cations. So, for a groundwater that contains both monovalent and divalent cations, there is not a rigorous CCC threshold below which bentonite will be vulnerable to sol dispersion.

SKB has instead derived an approximate safety function indicator criterion that is based on experiments with bentonite and solutions with mixtures of monovalent and divalent cations at varying concentrations (Birgersson et al. 2009). The derived criterion for bentonite to resist sol dispersion (safety indicator criterion R1c) is that the sum of charge equivalents of cations in interlayer solution, $\Sigma q[M^{q+}]$, should be >4 mM. This criterion is qualified by a requirement that the bentonite should have an exchangeable Ca content above 20% (SKB 2011, p 399). Bentonite in ion exchange equilibrium with 'typical' Forsmark groundwater is calculated to have approximately equal proportions of exchangeable Ca^{2+} and Na^{+}, but this would of course evolve as the groundwater compositions around deposition holes changed over time.

Salinity evolution in the regional-scale model of flow and transport is done in terms of per mil salinity or TDS (total dissolved solids) only. Therefore an approximation based on data from groundwater samples is used to relate the modelled salinity values to $\Sigma q[M^{q+}]$ values, and thus to assess the extent of groundwater dilution against the safety function indicator criterion of >4mM. The approximation is that this criterion of >4 mM is equivalent to >0.27 g/L TDS (SKB 2011, p 359).

2.2.3. Criteria for this assessment

My assessment is therefore concerned with how SKB has presented:

- Conceptualisation in general of how groundwater salinity might evolve in the future;
- Description of present-day salinity distribution at the site and potential origins and compositions of future dilute water infiltration;
- Initial state compositions for modelling of groundwater salinity evolution;
- Modelling of dilution of groundwater compositions in the repository system through an ongoing temperate climate;
- Modelling of further dilution of groundwater compositions through a future glacial climate;
- Modelling of the possibilities for dilute water penetration to deposition holes and into contact with buffer;
- Interpretation and modelling of the potential effects of water-rock reactions on dilute groundwater compositions;
- Other lines of evidence about long-term salinity evolution in crystalline rock groundwaters;
- Consideration of alternative concepts, models, parameters and scenarios.

SKB's conclusions on these aspects of salinity evolution can be evaluated in the context of what is required by the relevant safety function, in terms of either sum of cation equivalent concentrations or corresponding salinity.

2.3. Consultant’s assessment

2.3.1. Description of compositions of present-day groundwater and dilute water infiltration in the future

Present-day groundwater and pore water compositions

SKB’s description of present-day groundwater compositions and of the spatial distribution of salinities is well-established. Groundwater compositions have been interpreted with the M3 principal components analysis tool in terms of mixtures of reference waters. This approach to describing groundwater compositions in terms of mixtures of several components has been thoroughly tested by SKB for sensitivity to assumptions about reference water compositions, as described in section 2.1.2. My assessment of these aspects of site description is that the level of knowledge of groundwater compositions, their distribution and the sources of the different water components that constitute the present groundwater system is generally adequate as the basis for forecasting likely long-term evolution of salinity.

The paucity of groundwater compositional data for the target rock volume, the rock domain FFM01 at and below repository depth, is an issue but it is evident that this is accounted for by the difficulty of obtaining water samples in rock with low frequency and transmissivity of fractures. Data from the few water samples obtained plus the indications from pore water salinities do not indicate groundwater compositions that would be anomalous in terms of the general increase of salinity with depth. Indeed, they suggest a rather steeper gradient of increasing salinity through FFM01 which is consistent with the hydrogeological evidence for decreasing overall permeability and slower groundwater movement in that domain.

Data for compositions of pore waters in the rock matrix are sparse in terms of lateral distribution through the rock volumes of interest, but are relatively more frequent in the vertical borehole profiles where samples have been extracted and analysed. These data are adequate for salinity evolution modelling, although the uncertainties in the Cl^- concentrations are higher than for normal groundwater samples. Cl^- is the only one of the major solutes contributing to salinity that can be analysed meaningfully in pore waters, but the data give a sufficient indication that pore waters are generally slightly less saline than corresponding groundwaters.

Modelling of future salinity evolution depends on data for present-day groundwaters and pore water compositions in a number of ways.

Firstly, the interpretation in terms of mixing proportions of reference waters underpins the assignment of initial state water compositions in terms of reference water proportions for the regional-scale model of salinity evolution from a starting point in the past. This initial state and starting time for the model has been selected as the interpreted groundwater system at post-glacial and pre-Littorina time, i.e. about 10,000 years ago, as discussed in the next section. The rationale for this selection is presumably that the state and composition of the groundwater system can be reasonably well judged on the basis of it being at the end of a period of glacial melt water dominance and before the Holocene processes of Littorina seawater intrusion, land uplift and meteoric water infiltration.

Secondly, present-day compositions of groundwaters and pore waters are used to test the validity of, and to calibrate, the regional-scale model for salinity evolution. The model has a starting point in the past and therefore the first stage is a simulation of palaeohydrogeological evolution up to the present day, as explained in section 2.1.3. Modelled salinities (or TDS) and proportions of reference waters have been compared with measured water compositions for groundwaters and pore waters. In my opinion, this important step of model testing and confirmation is not well enough described in the main report of SR-Site, although I have been able to put together a reasonable and hopefully valid understanding of what has been done from other reports in SR-Site and previous stages of the programme. This is discussed in more detail in section 2.3.3.

Thirdly, an understanding of the present-day distribution of the component reference waters and of the way that the system responded to past climate changes with inputs of waters from different sources should be able to increase confidence in the boundary conditions and potential impacts on the system of future climate changes. In my view, SKB has achieved as much as possible out of these interpretations as reported in the supporting hydrochemical interpretation reports in SR-Site, SDM-Site and prior stages of the programme.

Dilute water infiltrating during a temperate period

Dilute water entering the groundwater system in bedrock fractures in the future could originate from a number of distinct sources:

- Vertical infiltration of meteoric precipitation, i.e. rainwater or snowmelt, at the land surface of the repository footprint above the target volume;
- Leakage of water through the base of lakes or Baltic sea and then vertical and lateral flow towards the target rock volume;
- Lateral flow of dilute groundwater, having meteoric origin, from bedrock elsewhere in the region along hydraulic gradients that will develop as land uplift progressively changes topography;
- Infiltration of dilute water that would originate from melting of an overlying or nearby ice sheet during a future glacial climate period;
- Out-diffusion of water from porewater in rock matrix adjacent to transmissive fractures (porewater is not dilute, but generally has lower salinity than nearby fracture water as explained in section 2.1.1 so diffusion will tend to have a diluting effect on groundwater).

Vertical infiltration of rainwater and snowmelt, i.e. 'meteoric water', at the surface then through soils and glacial sediments and into bedrock is an ongoing process. The water table position fluctuates in response to amount of infiltration but is likely to remain close to the surface throughout likely temperate climate conditions in the future. Evapotranspiration losses of water from soils and from lakes are so small that there will be negligible increases of salinity due to that process. When infiltrating water reaches the water table, it mixes with pre-existing water and will therefore become more mineralised, notably with higher Cl^- concentrations. Relatively rapid geochemical reactions also occur between infiltrating water and reactive mineral grains in soils and shallow bedrock. These reactions also increase the overall mineralisation of the water due to increases in concentrations of cations and of alkalinity, primarily bicarbonate anion. Sulphate, SO_4^{2-}, concentrations may also increase due to oxidation of sulphide minerals in soils, but Cl^- concentrations are not changed significantly because there are no minerals containing substantial amounts of Cl^- in soils and bedrock.

Shallow groundwater, below the water table, tends to move laterally under the influence of the hydraulic gradient of the water table. This behaviour, coupled with the enhanced hydraulic conductivity of shallow bedrock due to frequent sub-horizontal fracturing, constitutes what has become identified as a shallow 'aquifer' that extends perhaps to around 50 m depth. Diversion of infiltrating water as lateral flow, much of it presently to discharge into the seafloor or into lakes, means that only a small proportion of total infiltration continues downwards and ends up as recharge to deeper groundwater in the fracture network in bedrock.

Leakage from lakes and streams is a specific sub-model of infiltration. Lakes are supplied with dilute meteoric water by direct precipitation or by stream inflows. Close to the coast lakes may also contain a portion of seawater and thus be brackish. Whilst the shoreline is nearby, in the early future before land uplift has caused the shoreline to recede, leakage of Baltic seawater may also occur. Water infiltrating from lakes and sea may therefore range in composition from dilute to brackish. There is a possibility that leakage water from lakes and streams, essentially unaltered precipitation, may pass directly into bedrock fractures with less chance of mineralising reactions than happens with infiltration through soils. That may be one of the factors accounting for the variability in the total mineralisation of shallow groundwaters.

Lateral 'regional' flow of dilute groundwater from bedrock elsewhere in the region will probably come from further inland or wherever the topography is controlling the hydraulic gradient. This is a realistic concept for the origin of at least some of the non-marine groundwater that is currently in the target volume at Forsmark. Uplift due to post-glacial recovery is causing ongoing modification of topography and thus is changing the regional hydraulic gradient from inland towards the Baltic Sea. It is likely that the hydraulic gradient towards the Forsmark site will increase through the future temperate period and thus the lateral flux of dilute groundwaters into the target volume will also increase. Therefore the advance and rate of salinity dilution in the target volume should take account of this in addition to vertical infiltration. Relevant groundwater masses in the region inland from Forsmark have not been characterised, so there are some uncertainties in the potential effects on groundwater compositions.

The importance of the above discussion about sources of dilute infiltration during the temperate climate period is that these water sources will be driving the evolution of salinity towards more dilute concentrations as they infiltrate and flow deeper. Dilute infiltration will mix with the greater bulk of pre-existing, older groundwater and thus the progress of dilution in the bedrock system will be attenuated.

SKB has chosen to represent the most dilute end member in this dilution and mixing process with a reference water that is assigned the composition of a shallow bedrock groundwater, as discussed in section 2.1.2. The composition has 181 mg/L Cl^- which is considerably more than would be the concentration in unaltered meteoric water or recently infiltrated soil water. SKB has justified this 'altered meteoric water' composition as being a realistic approximation of the minimum mineralisation of recharging waters that enter the deeper groundwater system and mix with pre-existing groundwaters. For present purposes of forecasting salinity evolution through the temperate period, it is important to be confident about this and about SKB's implication that it is highly improbable that substantially more dilute water would exist in shallow bedrock and move towards repository depth.

It would be quite plausible for rather more dilute waters to occur in shallow bedrock at some time in the future, especially when dilute water infiltration has progressively flushed vestiges of brackish water from the shallow part of the system. Infiltration of less altered meteoric water might occur either through soils that have less reactive material (especially less organic material driving P_{CO2} and mineralising reactions) or directly from lakes. In any of those cases, Cl^- concentrations lower than 181 mg/L will probably occur. This is supported by low Cl^- concentrations in some of the groundwater samples from the Stripa mine and from the inland sites that were drilled by SKB's exploratory programme in the 1980's (although it is acknowledged that drilling water contamination may account for some dilution in these).

It is noted that SKB has done a rather intensive study of the sensitivity of the M3 PCA mixing calculations to the compositions that are assumed for the reference waters and has shown that there is a dependence on what is assumed for this reference water, not unexpectedly. It can be argued that, although the present 'altered meteoric' reference water might be suitable for palaeohydrogeological mixing calculations of what constitutes present groundwaters, a more dilute reference water should be used, at least as an alternative, for modelling of future groundwater salinity and hydrogeochemical evolution.

Most importantly, the altered meteoric reference water composition exceeds the safety function indicator criterion of $\Sigma q[M^{q+}]$ being >4mM, or the approximately equivalent salinity of 0.27 g/L TDS. So, in principle, modelling of groundwater salinity evolution due to flushing and mixing with this reference water as the only source of dilution will always give compositions that are acceptable by this criterion. Of course, SKB has recognised this and have done their key dilution modelling with an end member with zero salinity to test a 'worst case' of infiltrating water composition. Therefore the choice of dilute reference water composition is not a significant issue for the safety analysis. However SKB has taken a rather tortuous route to studying and reporting this issue in SR-Site.

Dilute water infiltrating during a glacial period

In contrast with the reference water composition for infiltrating meteoric water during the temperate climate, SKB has used a very dilute composition for the glacial melt reference water (Table 1). Cl^- concentration is 0.5 mg/L and total mineralisation is <0.3 mM. The sum of cation equivalents, $\Sigma q[M^{q+}]$, is <0.2 mM and is therefore lower than the safety function indicator criterion for buffer erosion, >4 mM.

Compositions of meltwaters in various glacial settings were compiled by R. Arthur (Appendix C8 in Robinson and Bath, 2011). Activity ratios a_{Na+}/a_{Ca2+} of the various melt waters were all much lower than the value of 0.05 which is the approximate upper limit for stability of bentonite as a colloidal gel. It corresponds to a value of 0.9 for the equivalent fraction for Ca^{2+} in exchangeable ion sites on montmorillonite.

The assigned glacial reference water composition is very dilute and does not satisfy either the a_{Na+}/a_{Ca2+} criterion or the performance indicator criterion set by SKB, $\Sigma q[M^{q+}]$. There are sparse data for present-day glacial melt waters and large irreducible uncertainties in any estimate for glacial melt water compositions for a future ice sheet over Fennoscandia. It is therefore prudent for SKB to assign a very dilute composition to be pessimistic in terms of this safety function criterion.

Anyway, for at least some of the simulations of salinity evolution both in temperate and glacial climates, SKB have made the very pessimistic assumption that infiltrating dilute water has zero salinity. It is not entirely clear which model runs had this boundary condition, but the difference between that and the glacial melt reference water composition is negligible. It is a different case for the model of salinity evolution in the temperate climate because the original boundary condition was set by altered meteoric water which already has a composition that satisfies the salinity and cation concentration requirements of the safety function criterion. SKB sensibly used the pessimistic zero salinity boundary composition instead of the altered meteoric water for at least some of the model runs.

The variability of shallow groundwater compositions through periglacial and glacial conditions may be large due to the effects of salt freeze-out as permafrost forms, but this is also uncertain. In any case, periglacial groundwaters are unlikely to be as dilute as glacial melt waters, so uncertainties about periglacial processes are not significant for the present purpose.

Effect on fracture water compositions of diffusive exchange with pore waters

Groundwater in fractures exchanges interacts with the larger quantities of older pore water in the intact rock matrix by out-diffusion. The general pattern at Forsmark is that pore water generally has lower salinity than that of current nearby fracture water so diffusive exchange will tend to have a diluting effect on groundwater. However saline groundwater would not be diluted to significantly low levels by this mechanism alone.

Probably of greater significance is the diffusive exchange between pore waters and infiltrating dilute groundwater at some time in the future. The process would tend to increase the mineralisation in the groundwater and thus attenuate the progress of very dilute water reaching repository depth. Diffusive exchange between water in rock matrix and water in a fracture is dependent on flow-wetted surface area and flow rate of water in the fracture, i.e. analogous to the mechanism of radionuclide retardation. Thus faster flow rate will tend to restrict the effect of diffusive exchange and higher flow-wetted surface will tend to promote diffusive exchange.

2.3.2. Initial state for modelling future evolution

The initial state of groundwater compositions at the starting point for modelling future salinity evolution has been set by SKB as described in section 2.1.2. The depth-dependent variations of groundwater and pore water compositions have been assigned in terms of proportions of reference waters. Initial conditions are an estimate of groundwater and pore water compositions at the end of the last glaciation. Initial conditions in footwall bedrock in terms of reference water proportions are set at 100% glacial water from 0-400 m depth and a binary mixture of glacial and deep saline waters from 400-1500 m, below which the composition is 100% deep saline water. Initial conditions in hanging wall bedrock are set to have deeper penetration of glacial water. These proportions of reference waters have been used in the regional-scale model but have been converted with the assigned reference water compositions to salinity values for DFN modelling.

I note that the inferred penetration of glacial water to 1500 m in these initial conditions is much deeper than interpreted in the Site Descriptive Model. Presumably this apparent inconsistency reflects the uncertainties inherent in the mixing model using reference waters. It is probably insignificant overall but SKB could acknowledge this and provide some discussion of how the various aspects of non-uniqueness in the use of reference waters for initial conditions and transport modelling propagate through the modelling. I suspect it has negligible effect because, if glacial and meteoric waters, recent or old, all have dilute salinities then which reference water is used to explain dilution is more or less irrelevant for the present purpose.

SKB do not discuss why they have run the ECPM model for future evolution of salinity using an initial condition in the past rather than the present-day compositions as initial condition. I assume that it has been done so that there the modelling is seamless between the palaeohydrogeological model calibrated with observed compositions and the model of future evolution.

An additional reference water, ‘old meteoric’ water, has been assumed for the description of the initial state at 10,000 years ago. This has the same composition as present-day meteoric water except for lower alkalinity and heavier stable isotopic ratio (Table 1). It differs from the ‘old meteoric + glacial’ end-member composition used in the hydrogeochemical interpretation. There is insufficient explanation of this difference, but I assume that the aim was to have a palaeohydrogeological component that is not itself a hypothetical mixture and that has a stable isotopic ratio that can account for the compositions of deep very old groundwaters. The lack of clarity in reference waters is hindered further by what I assume to be a typographical error in a table of definitions. Overall, however, I think that the ‘old meteoric’ reference water is a sensible assumption to account for the observed trend in stable isotope compositions and specifically to represent a likely initial state mixture of groundwater components that existed in the site after the last glaciation and before the influx of Littorina sea water. How this old meteoric reference water is defined affects the calculated proportions of glacial reference water, but it does not have a significant impact on how future salinity evolution is modelled..

The most significant question for present purposes is whether the initial state as assigned is a reasonable expert judgement and especially whether there is any argument for proposing a more dilute initial state for the modelling. Firstly, the depth-dependent proportions of the glacial and deep saline reference waters look reasonable, noting that glacial melt water is hypothesised to have penetrated to 1000 m depth in the footwall rock and 1800 m in the hanging wall rock (see discussion of this above). The corresponding proportions of old meteoric reference water are rather arbitrary and are really defined by the optimisation of M3 analyses of measured water compositions especially with respect to stable isotope composition. However the overall suitability of the selected initial state is best assessed in terms of the match to measured groundwater compositions that is given by modelling from initial state, at 10,000 y ago, to the present-day reference water proportions. In that context, the selected initial state looks suitable. Alternative initial states have not been used to assess the sensitivity of the modelled present-day compositions to assumptions about initial state, but in my judgement there will not be alternatives that would match the present-day compositions and also make significant differences to the long-term modelling of dilute water penetration.

2.3.3. Dilute water infiltration through the temperate period

My assessment is sub-divided under a number of themes: (i) Construction of the model; (ii) Initial conditions and boundary conditions; (iii) Duration of model simulations; (iv) Matrix diffusion and other transport properties; (v) Model testing and calibration; (vi) Model results for dilute water infiltration.

Construction of the model

SKB has modelled the infiltration of dilute water through both the temperate and glacial periods using the regional-scale ECPM model. The grid of the regional-scale model is too coarse for the simulations to be meaningful at the scale of deposition holes and anyway the repository tunnels are not represented in the ECPM model grid. The results are spatially averaged at the scale at which hydro DFN properties have been converted into ECPM properties, i.e. at the scale of the ECPM grid. The ECPM modelling uses a state-of-the-art numerical code and is well proven in previous stages of SKB’s programme as the most appropriate and valid approach to simulating the transport and mixing of natural tracers such as Cl^- and total salinity and of proportions of reference waters derived from statistical analysis of groundwater compositions.

The construction and parameterisation of the DFN, and whether there are alternative approaches to upscaling that would produce different properties in the ECPM, are outside the scope of my assessment. SKB states that confidence is high in the bedrock hydrogeological model, which I assume refers to the DFN model, and that there are greater remaining uncertainties in the properties of the deformation zones (DZs). Uncertainties in properties of the DZs propagate directly into the model outputs of salinity evolution at various times. More transmissive DZs would result in dilute groundwater advancing more rapidly than is suggested by Figures 2 and 3.

Solute transport and retardation through the ECPM regional-scale model should be essentially the same as it would be through the DFN that is nested within the ECPM and from which the ECPM has been parameterised. SKB have not, as far as I understand it, shown that that is the case. Salinity evolution and propagation of dilute water to depth would not be reliably modelled if, for example, the connectivity and anisotropy that are implicit in the DFN were not replicated by the ECPM. An additional issue is that solute transport pathways in larger fractures or channels would have lower flow-wetted surface areas than DFN fractures and thus would experience lower degrees of dilute water attenuation by diffusive exchange with matrix waters.

Solute transport and attenuation of dilute water penetration through the DFN models at site-scale and repository-scale are simplified processes that are simulated with particle tracking and an analytical formula for diffusive exchange with matrix pore waters. The details of SKB’s stochastic modelling that results in the forecasts of the number of deposition hole positions receiving dilute water are not always explained adequately. Perhaps there are aspects that are still not fully understood because there has not been enough sensitivity and variant modelling, although I appreciate that SKB has assessed various pessimistic scenarios. A key issue in this respect is the overall relative influences on SKB’s model calculations of the average numbers of deposition holes affected by dilute water of (a) DFN connections to individual deposition holes, (b) proximity to a nearby transmissive deformation zone, and (c) attenuation of dilute water composition by diffusive exchange with matrix water.

Initial conditions and boundary conditions

Initial conditions for the regional-scale model of salinity evolution from 10,000 y ago to present day have been assigned by expert judgement as discussed above in section 2.3.2. SKB's justification of the selected initial conditions is, in my judgement, has an appropriate degree of simplification. The validity of the assigned distribution and proportions of reference waters and salinities is confirmed semi-quantitatively by the comparison between modelled and measured fracture water and pore water compositions for the present day (see below). The match between modelled and measured compositions is also used for calibration of the ECPM model, so SKB has implicitly assumed for calibration of hydraulic and transport properties that the initial state compositions are valid. I think that this is reasonable.

Boundary conditions in terms of hydraulic conditions and infiltration composition are necessary simplifications of the likely complexity of future topographic conditions and water compositions. Uncertainties in the evolution of topographic and hydraulic conditions are likely to be less significant for present purposes than uncertainties in the hydrogeological properties of the DZs that will control salinity evolution and downwards penetration of dilute groundwater.

Compositions of water entering the system during future temperate and glacial periods are the 'altered meteoric' and 'glacial' reference waters respectively. Altered meteoric water has a $\Sigma q[M^{q+}]$ value of about 14 mM so it has higher mineralisation than the safety function indicator criterion of 4 mM. It is therefore impossible for modelled groundwater salinity to evolve through the temperate period to a $\Sigma q[M^{q+}]$ value lower than 4 mM. To address this, some runs of temperate and glacial climate evolutions have also been modelled with an input of zero salinity water as a pessimistic assumption for melt water composition.

I agree with SKB's general assumption that infiltrating water during the temperate period will achieve a composition that can be typified by the 'altered meteoric' reference composition. This is a rather fundamental aspect of forecasting dilute water penetration into the groundwater system because it presumes that groundwater, at least during the temperate stage, could never become so dilute as to fail to comply with the safety function criterion to prevent buffer erosion. However that possibility has not been entirely excluded from SKB's modelling because a zero salinity boundary composition pessimistically discounts the mineralising effect of hydrogeochemical reaction of dilute water in soil and shallow bedrock conditions.

The assumption of no lateral flow through the sides of the model is a further simplification. As land uplift proceeds through the initial temperate period, there will be an increasing tendency for lateral regional groundwater flow that will enter the target repository volume through the sides of the ECPM model domain. My inference in this respect seems to be supported by the fact that the DarcyTools hydrogeological model for glaciation effects allows for lateral flows.

SKB has not explained why lateral flows from outside the ECPM regional model boundaries would have a negligible impact on salinity evolution at repository scale, although it states that the hydrological impact of land uplift will extend beyond the boundaries of the regional model after about 10,000 years into the future. Has SKB investigated the sensitivity of the temperate period groundwater salinity model to this? Dilute groundwater from outside the inland boundary of the model will have the same hydrogeochemical processes affecting mineralisation so the impact of flow through the side boundaries of the model would be similar to the effect of increasing vertical infiltration.

Duration of model simulations

Simulations of salinity evolution and dilute water infiltration during the temperate period of the base case evolution have mostly been limited to a duration of 10,000 years into the future, starting from an initial state defined for 10,000 years ago (see above). The base case has a temperate period duration of 30,000 years and the variant scenario with an extended temperate period due to global warming has a duration of 60,000 years. Simulations to 10,000 years into the future are comprehensively reported and are consistent with the expected evolution of salinity on the basis of how the system evolved in the past from the pre-Littorina starting point 10,000 years ago. The durations of the simulations are rather inconsistent which is confusing – some go to 7,000 or 9,000 years in the future rather than 10,000 years, whilst the hydrogeochemical model simulations go to 7,000 years, but this does not substantially affect the value of the model results. In general, the results emphasise the dominant role of the major hydraulic conductors, the deformation zones, in transmitting dilute water downwards through the system.

The reporting of modelling for the extended temperate period is much less satisfactory in the sense that very little information is provided. It is unclear whether the extended duration model is identical to the 10,000 year model, or whether some changes had to be made to the basic model to run it for the much longer timescale. The very limited graphical illustration of results, just one cumulative distribution plot with a logarithmic timescale, allows only a simplistic comparison between model outputs for the two timescales.

A number of varying scenarios and timescale have been modelled for glacial melt water infiltration including infiltration under fully glaciated conditions for an extended timescale of 100,000 years. Another model variant has assumed glacial conditions for 25% of the 120,000 years duration of the next glacial cycle. These hypothetical scenarios are pessimistic simulations and therefore are adequate assessments of the maximum likely infiltration of dilute water, in my opinion.

Matrix diffusion and other transport properties

The regional scale model is the only one of the models at different scales to explicitly include a full coupling between advective flow and solute transport and matrix diffusion of solutes. Matrix diffusive exchange is the dominant process by which, in the long term, dilute water advance will generally be attenuated, so the regional model is important in this respect.

Uncertainties in measured pore water salinities have probably been underestimated, but nevertheless it is evident that pore water salinities could be a significant buffer of future salinity evolution in fracture waters. Pore waters are less saline than present-day fracture waters at repository depth, so the effect of matrix diffusion in the early stages of temperate climate evolution is to dilute fracture water compositions. As dilute water infiltrates and permeates the fractures, this is reversed and diffusive exchange will tend to increase the salinity of dilute water and thus attenuate the penetration of dilute water at later stages of the temperate and glacial climate periods. The overall effect of matrix diffusion on dilute water attenuation would depend on the efficacy of diffusive exchange between fracture waters and pore waters which, in turn, depends on advective water velocity, diffusivity, and the depth of diffusion-accessible porosity in the matrix.

SKB’s model for solute exchange between fracture waters and pore waters is simplified by assuming that the entire matrix is accessible by diffusion. For rock domain FFM01 in which transmissive fracture spacing is typically 25 m, the diffusion-accessible matrix depth is therefore about 12.5 m. The evidence to support this assumption is, in my opinion, scant although the evidence for any such limitation is also absent. If that assumption is invalid and the rock matrix is accessible only to a limited depth, then matrix exchange will be less effective at attenuating dilute water advance. If the values for solute diffusivity of the rock matrix or for flow-wetted surface area of fractures have been overestimated, it will have the same effect.

The sensitivity of dilute water attenuation by diffusive exchange with more saline pore water to the diffusion-accessible depth of matrix has not been reported in detail. However SKB state that this has been done and indicates that it is not a primary issue. It is likely that, even with a restricted depth of diffusion-accessible matrix, there will still be the capacity for diffusive exchange to have a significant effect on the salinity of water, i.e. to attenuate the degree of dilution. Similarly, uncertainty in the diffusivity of the connected pores in the matrix is unlikely to substantially affect the capacity to attenuate dilution.

Evidence that matrix diffusion will be a significant process in in the future evolution of salinity and attenuation of dilute water penetration comes from considering how present-day pore water compositions reflect diffusive exchange in the past. These data have been interpreted in terms of diffusion being effective for ‘several 10s of cm’ into the matrix, and as evidence that pore waters were dilute prior to the start of Pleistocene glaciations.

The value assigned to dispersivity in the ECPM model influences the transport of solutes and therefore the penetration and mixing of dilute water infiltration. Values have been assigned for both longitudinal and transverse mixing. It seems that a value of 50 m has been used for longitudinal dispersion length. SKB states that changing dispersion length from 40 to 50 m has negligible effect other than stabilising the numerical convergence. However, for a flow path length of around 500 m the choice of dispersion length could be significant for the degree to which dilute water has been attenuated by mixing towards repository depth. Uncertainty in the concept and parameterisation of dispersion means that the degree of dilution at repository depth could be over- or under-estimated. If the value is too high, the model will simulate too much dispersive mixing with pre-existing saline water and excessive attenuation of infiltrating dilute water. SKB could provide more explanation of how hydrodynamic dispersion is represented in the models at different scales and whether or not there is a significant dependence of dilute water mixing and attenuation on the choice of dispersion length.

Model testing and calibration

SKB has described how the hydrogeological properties of the regional-scale model have been calibrated against pumping test data and also calibrated against observed chemical and isotopic water by palaeohydrogeological modelling from 10,000 years ago to the present day. Vertical hydraulic conductivity was reduced by an order of magnitude to improve the fit to hydrochemical and interference test data. This approach to large-scale flow and transport properties looks as robust as can reasonably be achieved, though its limitations as a simplistic ‘curve matching’ comparison need to be taken into account in considering potential uncertainties.

The calibration has been possible only for the shallower part of the system, above -400 m, because availability of relevant data is less dense towards repository depth, especially for the target volume in fracture domain FFM01. SKB reports that the results (particle tracks, Darcy fluxes) from the site scale model are insensitive to the effects of calibration on the boundary conditions exported from the ECPM model to the DFN site scale model. DFN parameters at repository depth are not, anyway, affected by the calibration. Nevertheless it seems possible that the lower hydraulic conductivity suggested by calibration for shallower parts of the system might also apply at repository depth. That would decrease the calculated rate of dilute water penetration through the DFN and would have a relatively large impact on the penetration of dilute water towards repository depth along the major transmissive paths, the deformation zones. SKB note that there is a large degree of uncertainty in the hydrogeological properties of the DZs. Thus overall I conclude that there are relatively large remaining uncertainties in the ECPM representation of salinity evolution and the extent of dilute water penetration towards repository depth, as illustrated for example by the model output in Figure 2.

Another aspect of palaeohydrogeological evolution that could have been simulated and compared with present-day evidence is the penetration of glacial meltwater from the last glacial cycle. SKB has not reported any such palaeohydrogeological modelling, one argument being that the definition of initial state for such a model is extremely uncertain.

Model results for dilute water infiltration

SKB has modelled the infiltration of dilute water through both the temperate and glacial periods using the regional-scale ECPM model. The grid of the regional-scale model is too coarse for the simulations to be meaningful at the scale of deposition holes and anyway the repository tunnels are not represented in the ECPM model grid. The results are spatially averaged at the scale at which hydro DFN properties have been converted into ECPM properties, i.e. at the scale of the ECPM grid.

Diffusive exchange between fracture waters and pore waters in the rock matrix is potentially the most significant process by which the compositions of fracture waters in the future will be modified. Data from several borehole profiles indicate that pore waters consistently have lower Cl^- concentrations than nearby fracture waters. Uncertainties in pore water Cl^- concentrations from extraction tests have probably been underestimated, but nevertheless it is evident that pore water salinities could be a significant buffer of future salinity evolution in fracture waters. That would depend on the efficacy of diffusive exchange between fracture waters and pore waters which, in turn, depends on advective water velocity, diffusivity, and the depth of diffusion-accessible porosity in the matrix.

The regional scale model is the only one of the models at different scales to explicitly include a full coupling between advective flow and solute transport and matrix diffusion of solutes. Matrix diffusive exchange is the dominant process by which, in the long term, dilute water advance will be attenuated, so the regional model is important in this respect. Pore waters are less saline than present-day fracture waters at repository depth, so the effect of matrix diffusion in the early stages of temperate climate evolution is to dilute fracture water compositions. As dilute water infiltrates and permeates the fractures, this is reversed and diffusive exchange will tend to increase the salinity of dilute water and thus attenuate the penetration of dilute water at later stages of the temperate and glacial climate periods.

The model for solute exchange between fracture waters and pore waters is simplified by assuming that the entire matrix is accessible by diffusion (SKB 2010a, p 353).

For rock domain FFM01 in which transmissive fracture spacing is typically 25 m, the diffusion-accessible matrix depth is therefore about 12.5 m. The evidence to support this assumption is, in my opinion, scant although equally the evidence for any such limitation is also absent (see further discussion in ‘palaeohydrogeological evidence’ in section 2.3.7). If that assumption is invalid and the rock matrix is accessible only to a limited depth, then matrix exchange will be less effective at attenuating dilute water advance. If the values for solute diffusivity of the rock matrix or for flow-wetted surface area of fractures have been overestimated, it will have the same effect. The sensitivity of dilute water attenuation by diffusive exchange with more saline pore water to the diffusion-accessible depth of matrix has not been illustrated. However SKB state that this has been done and indicates that it is not a primary issue. It is likely that, even with a restricted depth of diffusion-accessible matrix, there will still be the capacity for diffusive exchange to have a significant effect on the salinity of water, i.e. to attenuate the degree of dilution. Similarly, uncertainty in the diffusivity of the connected pores in the matrix is unlikely to substantially affect the capacity to attenuate dilution.

Sensitivity of exchange with matrix pore waters to the value of diffusivity for matrix diffusion is indicated by the fact that SKB reduced the matrix diffusivity value from 10^{-13} to $4x10^{-15}$ m^2s^{-1} between SR-Can and SR-Site. SKB could clarify the background to this change. A higher value would anyway increase the rate at which dilute infiltration would be attenuated by exchange with more saline pore waters, so SKB’s modification of diffusivity is conservative with respect to dilute water penetration. This modification also has implications for radionuclide retardation.

The outcome of the regional-scale modelling of salinity evolution is also sensitive to other features, assumptions and simplifications in the model.

(i) Hydraulic and solute transport properties and their heterogeneity at repository depth in the ECPM model are upscaled from DFN properties. The construction and parameterisation of the DFN, and whether there are alternative approaches to upscaling that would produce different properties in the ECPM, are outside the scope of my assessment. SKB states that confidence is high in the bedrock hydrogeological model, which I assume refers to the DFN model, and that there are greater remaining uncertainties in the properties of the deformation zones (DZs). Uncertainties in properties of the DZs propagate directly into the model outputs of salinity evolution at various times. More transmissive DZs would result in dilute groundwater advancing more rapidly than is suggested by Figures 2 and 3.

(ii) Initial conditions for the regional-scale model of salinity evolution from 10,000 y ago to present day have been assigned by expert judgement as discussed in section 2.3.2. The validity of the assigned distribution and proportions of reference waters and salinities is tested by the comparison between modelled and measured fracture water and pore water compositions for the present day. This comparison is also the basis for calibration of the ECPM model, so there is a degree of compromise between confirming that initial hydrochemical conditions are appropriate and adjusting hydraulic properties.

(iii) For the model of future evolution, the boundary conditions in terms of hydraulic conditions and infiltration composition are necessary simplifications of the likely complexity of topographic conditions and water compositions. The assumption of no lateral flow through the sides of the model is a further simplification. Uncertainties in the evolution of topographic and hydraulic conditions are likely to be less significant for present purposes than uncertainties in the hydrogeological properties of the DZs that will control salinity evolution and downwards penetration of dilute groundwater. SKB has not explained why lateral flows from outside the regional model boundaries would have a negligible impact on salinity evolution at repository scale, although it states that the hydrological impact of land uplift will extend beyond the boundaries of the regional model after about 10,000 years into the future. Dilute groundwater from outside the inland boundary of the model will have the same general soil zone reactions increasing mineralisation so the impact of flow through the side boundaries of the model would be the same as increasing vertical infiltration.

(iv) The value assigned to dispersivity in the ECPM model influences the transport of solutes and therefore the penetration and mixing of dilute water infiltration. It seems that a single value of 50 m has been used. SKB argue that the sensitivity of the model to the value is negligible. A dispersion length of 50 m might have an effect on the degree to which dilute water has been attenuated by mixing towards repository depth. Uncertainty in the concept and parameterisation of dispersion means that the degree of dilution at repository depth could be over- or under-estimated. If the value is too high, the model will simulate too much dispersive mixing with pre-existing saline water and excessive attenuation of infiltrating dilute water. SKB should provide more explanation of how hydrodynamic dispersion is represented in the models at different scales and justification of the values assumed for dispersion length.

SKB has described how the regional-scale model has been tested and calibrated by palaeohydrogeological modelling from 10,000 years ago to the present day. There are several other aspects of palaeohydrogeological evolution that could also be simulated and compared with present-day evidence:

- Infiltration of Littorina water;
- Penetration of glacial melt water from the LGM;
- Heterogeneity (compartmentalisation?) of water compositions between major fractures (e.g. sub-horizontal fracture zones) and minor fractures;
- Exchange of solutes and isotopes between fracture water and matrix pore waters.

It would be useful to get SKB’s response on whether these types of simulations have been attempted or whether they are impracticable or of no meaningful value.

2.3.4. Dilute water infiltration through a glacial period

A future glacial period will probably start after a prolonged period of temperate climate evolution of groundwater compositions. Therefore the initial salinity of groundwaters at repository depth at the start of the glacial period has been assigned a value of 3 g/L TDS for regional-scale modelling of salinity evolution. Modelling of salinity through the prolonged temperate period indicates that it would probably be much less than 3 g/L, so I wonder if this value has been taken from the relatively short temperate period in the reference evolution. Temperate conditions in the reference evolution last for only 30,000 years in the future, and have been modelled to only 10,000 years in the future. The global warming variant has 60,000 years of temperate conditions. SKB should clarify the reasoning behind the choice of 3 g/L and explain how the model results would be affected by assigning a lower initial salinity that would be representative of the evolution at the end of a prolonged period of temperate climate.

There is of course large uncertainty in how groundwater compositions will have evolved by that stage of the glacial cycle. The only sources of dilute water infiltration to the system in the long term are meteoric water and ice melt. All other potential sources of infiltration at various phases of the glacial cycle will be more saline, e.g. seawater, and climate-related sub-surface processes such as permafrost and enhanced evapotranspiration will tend to make groundwater more mineralised.

Upconing of deeper groundwater, as is suggested for some parts of the groundwater system in the vicinity of the edge of an ice sheet, will also tend to make groundwater at repository depth more saline.

Water-rock reactions will increase the mineralisation of infiltrating melt waters, as explained in Bath (2011). In my opinion, SKB's assumption of the composition for glacial reference water and modelling of the evolution of melt water compositions by water-rock reaction are likely to underestimate the increase of mineralisation in this water, prior to mixing with pre-existing groundwater components.

SKB presumes that infiltration of dilute melt water from an ice sheet during a future glaciation will occur most intensively at the times when the ice front is advancing and retreating over the site. The assumed conceptual model of ice sheet hydrology has the downwards hydraulic gradient and resulting water flux at a maximum when melt water underneath the ice sheet is pressurised by the load of the overlying ice. Groundwater discharge would occur in areas where ice cover is absent, although permafrost might inhibit this. This conceptual model is a hypothesis for how melt water might infiltrate bedrock. It supposes that there would be a transient high flux of melt water into bedrock, lasting only as long as it would be promoted by a high differential hydraulic gradient between downflow at that point and upflow elsewhere. That is the basis of SKB's argument that melt water infiltration will occur only over a period of tens to hundreds of years as the edge of an ice sheet might advance or retreat over the site. While the region is completely covered by an ice sheet, SKB's concept envisages no significant infiltration to the bedrock. There would not be a local spatial differential in vertical hydraulic gradients and no capacity deep in the bedrock for high lateral fluxes on a large scale.

This is more or less the current paradigm for sub-glacial hydrology, though the evidence to support it is sparse and rather incoherent. Therefore I think it is sensible and precautionary for SKB to have made a supplementary calculation for the case where a small flux of sub-glacial water infiltration continues for a much longer period.

Ice sheet hydrology is an active area of research at present. SKB, Posiva and NWMO Canada have a dedicated programme of drilling and testing in Greenland (the 'GAP' Greenland Analogue Project) and there are various studies of melt water within and at the base of ice sheets, including studies of sub-glacial lakes. However coherent and reliable data for hydraulic gradients and net groundwater fluxes, and compositions, at various depths in bedrock at different locations under ice sheets have not yet been reported. Precautionary 'worst case' model calculations of sub-glacial infiltration have been done by SKB and they satisfactorily prove that, at least as far as the dilute composition of melt water and sub-glacial hydraulics are concerned, the safety analysis is robust to the degrees of uncertainties.

As for dilute water infiltration during a temperate period, SKB's regional-scale model includes diffusive exchange with pore waters in the rock matrix as a potentially major process that would attenuate the advance of dilute water into the system. The initial condition for pore water salinities at the start of the model for glacial melt water infiltration is also 3 g/L TDS, i.e. in equilibrium with fracture water salinity, so the effect of diffusive exchange is to attenuate the advance of dilute fracture waters. A more dilute initial salinity for pore waters would have a lesser effect. Diffusive exchange with pore waters in the DFN models is simplistically simulated with an analytical formula, without any restriction on accessibility of the matrix to exchange. The analytical formula presumably uses the transport resistance (‘F’) for fracture pathways calculated in the DFN. It seems that SKB has not evaluated the sensitivity of the dilute water penetration model to uncertainty and variability in F values. SKB does not offer any expert judgements on this matter. The relationships between the vulnerability of flow paths and deposition holes to dilute water penetration and the magnitudes of calculated F values are shown by SKB to be rather complex. This may be significant because diffusive exchange is the only process that attenuates dilute water. Further investigation and explanation of this would increase confidence that the uncertainties are secondary.

SKB’s base case model of glacial melt water infiltration assumes that the maximum duration for which groundwater movement to deposition holes will be enhanced by an ice sheet in the vicinity of the repository footprint will be 100 years. This is an expert judgement based, I think, on ‘typical’ rates of glacier advance and retreat but there are likely to be reasonable possibilities that this duration might be exceeded. SKB’s model indicates that, in the 100 year melt water ‘episode’, 147 holes would experience water that has been diluted to less than 0.3 g/L TDS (i.e. more dilute than the $\Sigma q[M^{q+}]$ criterion of 4 mM). If the ice sheet were to halt for only 20 years, the model estimates that 77 deposition holes would be affected, and conversely the ‘possible but unlikely’ longer melt water episode would give >150 holes affected. A variant DFN model with extended spatial variability gives slightly lower numbers of affected deposition holes: 99 and 44 respectively (Joyce et al., 2010, p 178). The limited scope of DFN realisations and variants that have been modelled suggests that, taking a qualitative view of the large uncertainties in virtually all aspects of glacial and sub-glacial processes, the number of deposition holes affected might exceed SKB’s deterministic estimate by several times, perhaps up to 500. I have the impression that the key determinant of which deposition holes are ‘at risk’ of dilute water penetration is the distribution and properties of DFN fractures, although SKB do not state this conclusion explicitly. SKB has not provided a convincing argument that the uncertainties in DFN fracture representations are constrained by the presented DFN variants.

In view of the uncertainties about sub-glacial hydrology, I think it is prudent for SKB to have considered an additional glacial concept whereby slower infiltration of melt water throughout the period of glaciation, i.e. for many thousands of years, should be considered. The model indicates that total ice sheet cover would have to continue for 100,000 years to get a similar proportion of deposition holes being affected (Figure 8). Although the boundary conditions for this calculation are only an illustration, this result addresses any concern that this might be a variant with more severe implications than the reference evolution.

An additional, pessimistic, illustration of risk is the estimate that deposition holes with the highest groundwater flow rates could be exposed to dilute water for 30,000 years of the 120,000 years period of a full glacial cycle. From this, SKB forecasts that only one deposition hole will actually experience a combination of flow velocity and water dilution of such severity that buffer will be eroded to the point of reaching advective conditions at the canister surface. Similarly, it is forecast that 23 deposition holes could suffer advective conditions in 1 million years. The assumptions implicit in this estimation, especially the role of water flow velocity in contact with the buffer, have not been explained. It is unclear how this conclusion compares with the other illustrative calculations of 'number of deposition holes receiving dilute water'. However, taking the various illustrations at face value, the probability of buffer erosion by dilute water looks very low. There would be greater confidence that this conclusion is valid if SKB could make a clearer case for the validity of the DFN representation of fracturing and transmissivity around deposition tunnels on which the conclusion seems to be dependent.

2.3.5. Dilute water penetration to deposition hole positions

In SKB's repository-scale hydrogeological DFN model, dilute water penetration to deposition holes is primarily controlled by the distribution of transmissive fractures that intersect deposition hole positions. Presumably, deposition holes that are not intersected by such a fracture have water and solute movement modelled solely in terms of diffusion through the intact rock matrix around the deposition hole position. This is not explicit in SR-Site, to my knowledge, and SKB should clarify and expand information about the conceptual model and the assumed processes for water and solute movement in the hydro DFN model. If my assumptions are correct, timing of penetration of dilute water to the deposition hole position depends on (a) advection of dilute water to the nearest transmissive fracture, and (b) time for diffusion of the 'dilute water front' through the rock matrix.

These issues are of paramount importance for the issue of dilute water penetration to deposition holes because the overall outcome of the modelling seems to be that dilute water will only penetrate to deposition holes that are intersected by a transmissive fracture in the hydro DFN model, regardless of how dilute the groundwater at repository depth is forecast to become by the ECPM regional model. The rate of increase in the number of deposition holes receiving dilute water as the timescale increases supports this perception.

A deposition hole that is not intersected by a DFN fracture will have water ingress to it limited by diffusion through the rock matrix. Characteristic times for diffusion through rock matrix are in the orders of 10^3 years for 1 metre distance and 10^5 years for 10 metres, depending on the values assigned to pore diffusivity and diffusion-accessible porosity. Therefore deposition holes that are separated from the nearest fracture by at least 10 metres or so of intact rock are likely to be effectively immune from external dilute water influence. In those cases, the hydrochemical environment of a deposition hole will be determined initially by any introduced water during construction and emplacement, including pore water in bentonite buffer, and then in the long term by pore water in the rock matrix. The corollary of these conditions is that the completed emplacement of canister and buffer will have a prolonged resaturation period which introduces another set of uncertainties about future evolution of the system.

SKB's forecasts of the number of deposition holes that would have advective groundwater inflows and buffer erosion obviously has some dependence on the correspondence of deposition hole positions to fracture positions in the DFN. It is not clear how the small number of realisations in the DFN model can give a stochastically valid representation of possible fracture intersections at remaining deposition hole positions after application of FPC/EFPC.

My understanding is that HRD bedrock between DFN fractures is assumed by SKB to be unfractured and thus to transmit water only by diffusion. SKB does not provide a complete conceptual description of this ‘unfractured’ rock that will surround most of the deposition holes, so I am uncertain about whether and how, given sufficient timescale, dilute water might eventually get into contact with buffer. Does it contain micro-fractures that transmit water very slowly, above a purely diffusive threshold but below a threshold of advection that would be significant in terms of buffer erosion and radionuclide transport? If the fabric of intact bedrock is below the diffusion threshold, then where does water for resaturation of buffer come from, and what are the implications of that for water composition and flow velocity?

The potential implications and validity of adding micro-fracturing into the conceptual model of the DFN and of representing this by enhanced diffusivity of rock around deposition holes could be explained. In my opinion, SKB’s reporting does not provide a sufficiently high degree of confidence that the conceptual model for water and solute transport and diffusion in the rock around deposition holes, typically over a distance scale of 10 metres or so, is a conservative representation of all possibilities for behaviour in the actual bedrock system. I do not have the expertise to comment in more detail on the DFN modelling or to make a quantitative assessment of the implications for confidence in long-term safety.

My judgement about the overall impact of these uncertainties in the hydrogeological DFN model on the probability of the buffer safety function being compromised by dilute water is that the DFN issues are secondary because of the dominance of processes by which dilute infiltration will be mineralised and mixed, as discussed in previous sections.

In other words, there is a very high probability that dilute water will penetrate to repository depth, especially if a prolonged temperate period were to prevail and, if not during that period, then during a subsequent glaciation. Transport through DZs, with relatively higher transmissivities, will account for that as SKB has made clear in the ECPM regional-scale modelling. However there is also a very high probability that the dilute water will have become mineralised sufficiently due to mineral dissolution reactions, and at least in the early stages of evolution mixed with pre-existing brackish groundwaters and exchanged diffusively with brackish pore waters, that the safety function indicator criterion of $\Sigma q[M^{q+}]>4$mM will remain compliant. The few deposition holes with intersecting transmissive DFN fractures, assuming that FPC/EFPC selection criteria have been implemented successfully, will receive water flowing in the connected DFN from the nearest DZ, as SKB’s repository-scale modelling indicates. It is highly probable that the inflowing water will, however, not have retained its original dilute composition and will therefore satisfy the requirement for maintaining buffer stability.

There are a number of approximations or simplifications and causes of uncertainties in simulations of water flow to deposition holes for which SKB does not evaluate the impact on model outputs. These are probably issues of secondary impact on modelling of dilute water penetration to deposition holes but some clarifications would improve confidence.

(i) Changes of salinity and density are not coupled with changes of groundwater heads in the DFN site-scale and repository-scale models. The DFN model does not model salinity evolution forwards in time so the initial state of salinity/density remains invariant. Boundary conditions are taken from the ECPM regional-scale model. At each time step, the DFN model calculates steady-state flow in a fixed salinity/density field. This flow field and the DFN are then used to generate particle tracks and corresponding transport resistance. Infiltration is modelled in the DFN by backwards tracing of particle tracks from deposition hole positions to surface. Therefore changes of salinity in the DFN model are driven by two model processes: advection from the boundaries and diffusive exchange with pore waters. Diffusive exchange is modelled with an analytical formula that incorporates the transport resistance. As the salinity evolves to less saline/dense compositions, the downwards hydraulic gradient is likely to increase, so this lack of coupling between salinity and heads is non-conservative. The effect is probably negligible, in my judgement, but SKB should confirm this with a quantitative analysis.

(ii) There are only 10 realisations of the base case probabilistic hydro DFN model, and fewer for some variants. This may be insufficient to bound the resulting stochastic uncertainties reliably. In that case, the probabilities of dilute water breakthrough at deposition holes could be lower or higher than estimated with the reported modelling. In general, I wonder if the full range of uncertainties in the DFN model for transport and salinity evolution has not been established because of the restricted conceptualisation of the DFN, although scoping calculations of the effects of channelling are referred to in SR-Site (SKB 2011, p 138). This aspect of site-scale and repository-scale modelling is outside my expertise, but in my opinion it is not clearly or fully explained in SR-Site. These uncertainties would be propagated into velocity of groundwater flow through the DFN, flow-wetted surface, and dispersion. Uncertainties in flow-wetted surface parameter would affect transport resistance and thus diffusive exchange as a process that attenuates the advance of dilute water. Longitudinal dispersion in the DFN appears to be discounted in SKB’s model or allowed for only by modelling multiple flow paths (SKB 2010a, p352).

(iii) SKB’s model of dilute water access to deposition holes focuses on the ‘Q1’ pathway, i.e. a bedrock fracture that intersects the periphery of a deposition hole. Comparable modelling of the ‘Q2’ (via EDZ) and ‘Q3’ (via deposition tunnel backfill) pathways to the buffer cap at the tops of deposition holes is not presented in SR-Site. How are the Q2 and Q3 flows partitioned between deposition holes? SKB should confirm that these pathways would be relatively insignificant for dilute water inflow.

(iv) The probability of deposition holes experiencing dilute water inflows is dependent on how the models at different scales connect and make flow paths. There are likely to be assumptions and simplifications in how the DFN fractures connect with DZs and how this affects the particle tracking from near-surface to deposition holes and vice versa. How does upscaling of the DFN affect connectivity through the DFN and from DFN to deformation zones? How does the DFN couple with the DZs including sub-horizontal fracture zones (e.g. A2) in the site-scale model?

2.3.6. Effect of water-rock reactions on groundwater compositions

SKB has assumed in the site descriptive model for Forsmark that the concentrations and relative proportions of major solutes are primarily determined at these sites by mixing of groundwater components from various sources (SKB 2008a). Mixing is certainly the primary process accounting for salinities and overall mineralisation.

However deviations from expected mixing relations for some of the hydrochemical parameters (Figures 6-5 and 6-10 in Salas et al., 2010) indicate that cation concentrations are also affected by dissolution reactions of calcite and aluminosilicate minerals and by cation exchange reactions. The significance of cation composition of groundwaters at repository depth is that the ratio of divalent to monovalent cations, $[Ca^{2+}+Mg^{2+}]/[Na^{+}]$, in groundwater influences the colloidal stability or dispersion of the bentonite buffer. The relative proportions of divalent to monovalent cations, as well as the total of cation concentrations, is in the background to definition of the compliance criterion for the safety function indicator $\Sigma q[M^{q+}]$ for water coming into contact with buffer.

Cation exchange with secondary clay minerals and reactive surfaces of other minerals could be modelled if data for cation exchange capacity, exchangeable cation occupancies on exchange sites, and equilibrium constant for cation exchange were available. However in reality the complete set of cation exchange characterisation parameters is not easily measured and has large uncertainties. Theoretical modelling of cation exchange with single minerals may be possible using *ab initio* values for parameters, but would not be routinely applicable and reliable for the present purpose. The only practicable way to represent cation exchange in a hydrogeochemical model for future groundwater evolution is to assume the cation exchange equilibrium parameters and then to assume that the present cation distribution among exchange sites is in equilibrium with the present groundwater composition.

This is how cation exchange was modelled in a study of the possible directions of hydrogeochemical evolution of dilute water (Bath 2011). The conclusion drawn from that modelling study is that the geochemical evolution of dilute waters penetrating towards repository depth could in theory result in groundwater compositions at repository depth that are depleted in Ca^{2+} and Mg^{2+} relative to Na^{+}. This reaction modelling has various uncertainties, e.g. thermodynamics, kinetics and cation exchange coefficients. The great majority of alternative reaction paths however resulted in cation proportions and concentrations that would not compromise the stability of bentonite buffer, according to SKB’s criteria. This is supported by hydrochemical observations suggesting that compositions of groundwaters in crystalline rocks that remain dilute are unlikely to evolve towards strong depletion of divalent cations (Frape et al. 1984, 2005; Nurmi and Kukkonen 1986; Pearson 1987; Gascoyne and Kamineni 1994; Laaksoharju et al. 1999, 2008; Iwatsuki and Yoshida 1999; Gascoyne 2004; Iwatsuki et al. 2005; Follin et al. 2008).

2.3.7. Other considerations

Groundwater compositions in crystalline rock at other sites

General support for a conclusion that dilute water, with $\Sigma q[M^{q+}]$ below 4 mM, is extremely unlikely to penetrate to repository depth during a prolonged temperate period can be derived from data for other bedrock groundwater systems at around 500 m depth and in various climatic and hydrogeological settings.

There are not many comparable investigations so the evidence is not particularly strong, but to my knowledge there are no cases of groundwaters with this level of dilution in crystalline rock at 500 m depth. Inland sites, i.e. without post-glacial seawater infiltration, in settings that both have and have not experienced Quaternary glaciations are of relevance. Such sites can be found elsewhere in Sweden and in Finland, Norway, France, Germany and other parts of central Europe, and also in Canada and USA.

The origins of salinity in deep groundwaters in crystalline Fennoscandian Shield rocks, i.e. whether from seawater or from deep geosphere sources such as water-rock reactions and fluid inclusions, has been a much-studied topic in the Swedish and Finnish programmes for many decades, and has similarly been investigated in the Canadian and UK programmes (Frape and Fritz 1987; Frape et al. 2005; Gascoyne 2004; Lahermo and Lampén 1987; Nurmi and Kukkonen 1986; Nirex 1997).

The palaeohydrogeology of movements and mixing of distinct groundwater masses, i.e. the responses of the deep groundwater system to past changes of boundary conditions such as inundation of the surface by sea water and glacial melt water intrusion, is more important in this respect, however, than water-rock reactions. Water-rock reaction has not been identified in general as a major source of salinity in crystalline rocks. Crystalline rock does not in general contain the ‘evaporite’ minerals, halite (NaCl) and anhydrite ($CaSO_4$), which can be sources of increasing salinity in sedimentary rock groundwaters.

Water-rock reaction can, however, be an indirect source of salinity in crystalline rock by releasing saline water from fluid inclusions. This was a much-debated process in the interpretation of hydrochemistry of groundwaters at the Stripa mine in central Sweden (Nordstrom et al. 1989). Mass balance scoping calculations suggested that only a small proportion of the inclusions in quartz and calcite would need to be leached to account for the chloride content of groundwaters in fractures (though it is unclear whether this mass balance took into account the time-dependence due to groundwater circulation, infiltration and continual replenishment of salinity). Mass balance calculations for other crystalline rock groundwaters, including those at the Äspö HRL, have been interpreted as evidence that fluid inclusions could not be the dominant sources of chloride for higher salinity groundwaters, e.g. at Äspö) (Savoye et al. 2004).

Water-rock reactions in crystalline rocks, in some geological settings at least, might also contribute directly to salinity through the dissolution of biotite. Biotite can accommodate small amounts of chloride in its crystal structure, replacing hydroxyls. The clearest evidence for this source of salinity being significant is in the Carnmenellis granite in southwest England. This conclusion was supported by geochemical analyses of biotite, experimental studies on biotite dissolution, trace element associations and geochemical modelling (Edmunds et al., 1984). It was proposed that the alteration probably involved chloritisation of hydrothermal biotite by acidic hydrolysis (Edmunds et al. 1985).

There is no evidence in SKB’s investigations at Forsmark to suggest that either fluid inclusion leaching or biotite hydrolysis are significant processes in terms of increasing the salinity of dilute groundwater as it infiltrates the system. The overwhelming weight of evidence indicates that the dominant sources of salinity are modern Baltic water (in very shallow groundwaters), Littorina water and a deep saline groundwater. The origin of salinity in the latter is itself a topic of conjecture. It is undoubtedly very old water and appears to be more or less ubiquitous in the Fennoscandian Shield, and also the Canadian Shield. Various hypotheses for its origin exist, i.e. residual metamorphic or hydrothermal fluid (cf fluid inclusions) perhaps mixed with very old, stagnant, meteoric water, or ancient seawater from precursor sedimentary rocks, or Palaeozoic basin brines that infiltrated from overlying sedimentary rocks that have since been eroded away.

The origin of the deep brine (or saline water, depending on level of salinity) at Forsmark is immaterial for present purposes, but the hydraulic conditions driving any movement of it, e.g. upconing, during future evolution of the site are relevant to the topic of whether dilute water could reach repository depth and how dilution might be attenuated by mixing with more saline groundwater.

Palaeohydrogeological evidence of groundwater salinities at repository depth

Palaeohydrogeological evidence of hydrochemical evolution, specifically whether dilute groundwaters have previously penetrated to repository depth, requires a large degree of expert judgement in its interpretation.

Secondary minerals in transmissive fractures, typically calcite, clays and iron oxides, might be indicative of groundwater compositions, water sources and water-rock reactions when they were precipitated (Degnan et al. 2005). For example, the morphology, or crystal shape, of a secondary mineral, e.g. calcite, may indicate the hydrochemical environment in which the crystal grew (Milodowski et al. 1997). $^{18}O/^{16}O$ in discrete growth zones of calcite is potentially an indicator of the proportions of glacial melt water to have penetrated to repository depth in past glaciation episodes, though the interpretation requires an assumption about the maximum deviations of past temperatures in deep groundwaters.

SKB has made a reasonably intensive programme of sampling and analyses (mineralogical, geochemical and isotopic) of the secondary minerals that occur in fractures in Forsmark rock (Section 2.1.1; SKB, 2008a). The dominant minerals are chlorite, calcite, laumontite/epidote/prehnite, pyrite and Fe-oxides. Stable O and C isotope analyses have been done on calcite. The only significant, for the present purpose, conclusion to be drawn from these data is that secondary calcite does not seem to have undergone any leaching episodes (SKB, 2008a, pp 325-328). This indicates that groundwater under-saturated with calcite has not circulated since deposition of the calcite which is thought to have occurred from 100s of millions of years ago up to the present. Calcite under-saturation is expected only in very dilute infiltration that had not experienced any water-rock reaction or mixing with pre-existing groundwaters, so the calcite evidence is fairly strong support for the absence of dilute water penetration in the past and specifically during the glacial episodes.

Evidence that matrix diffusion will be a significant process in the future evolution of salinity and attenuation of dilute water penetration comes from considering how present-day pore water compositions reflect diffusive exchange in the past (Section 2.1.3). These data have been interpreted in terms of diffusion being effective for several 10s of cm into the matrix, and as evidence that pore waters were dilute prior to the start of Pleistocene glaciations. The interpretation that pore waters further from fractures might be indicative of salinities of much older groundwaters, more than a million years ago, is, in my opinion, inconclusive. It is valid to infer from pore water salinities that there has been dilution at some time in the past relative to the deep saline water and the present measured groundwater composition. Whenever that relatively more dilute water evolved, the diluting water must have been present in adjacent fractures for longer than present groundwater and previous Holocene waters have resided in the system. Otherwise evidence of it would have been erased by subsequent diffusive exchange, as has happened to pore waters in more fractured shallow bedrock and in hanging-wall rock down to several hundred metres depth around the major deformation zones.

I conclude that the pore water evidence, though indicating past groundwater circulations that were more dilute than present in both footwall rock (the repository target volume) and hanging wall rock, shows that past groundwaters in the timescale of interest were always sufficiently mineralised (by mixing ± water-rock reactions) to be consistent with bentonite stability.

3. Consultant's overall assessment

3.1. General issues

As an introduction to this overall assessment, I comment on the organisation and clarity of SKB's reports for SR-Site and my experience in understanding SKB's methods and results and in accomplishing my assessment. My comments especially concern the challenge of finding coherent information about the concepts, parameters, simplifications and assumptions, modelling results, uncertainties and sensitivity tests and of understanding the rationale of SKB's arguments.

SKB's documentation of the long-term safety case SR-Site (SKB 2011) is a well-structured, internally consistent and reasonably comprehensive account of the modelling inputs and outputs plus other arguments. However detailed understanding and assessment of what has been done for salinity evolution and groundwater flow at repository depth has involved a considerable amount of searching through the supporting SR-Site documents and also some prior reports describing modelling developments between SR-Can and SR-Site.

The supporting SR-Site reports are the Groundwater Flow Modelling Methodology report (Selroos and Follin 2010), Data report (SKB 2010a) and the Hydrogeochemical Evolution report (Salas et al. 2010). Other reports primarily cover Hydrogeological Conceptual Model Development and Numerical Modelling using CONNECTFLOW, Stages 2.2 and 2.3 (Follin et al. 2007 and Follin et al. 2008), Groundwater Flow Modelling of Periods with Temperate Climate (Joyce et al. 2010); and Groundwater Flow Modelling of Periods with Periglacial and Glacial Climates (Vidstrand et al. 2010). There are also the Site Description Report, SDM-Site Forsmark (SKB 2009), report on Water-rock Interaction Modelling and Uncertainties of Mixing Modelling (Gimeno et al. 2008) and the corresponding Confidence Assessment report for SDM-Site (SKB 2008b).

Although the evolution of salinity and penetration of dilute water to repository depth and deposition holes is a primary issue in SR-Site, there is not a comprehensive single account of how the modelling of this phenomenon is tackled. It is evident, I think, that the modelling of groundwater flows and solute transport and exchange with matrix have been 'work in progress' right up to the delivery of SR-Site. That has made it difficult to get a picture of exactly how the models are constructed and what the assumptions and input parameters are. Sometimes, key inputs and outputs are difficult to find and have been reported in slightly different ways across reports.

I appreciate that modelling of groundwater flows and solute transport in a fractured rock medium, and consequent evolution of water compositions, far into the future through changing climate episodes are complex challenges. The required models and parameter choices are sophisticated and involve complex justifications. I have found it difficult to achieve an understanding of what has been done that is sufficient to give me confidence in the representation of the system and in the modelling outputs.

A new synthesis of this specific topic could provide a coherent and logical account of what has been done, explains how the modelling requirements at different scales of space and time have been achieved, compiles all of the input data and relevant output data, and illustrates the model outputs at appropriate scales. This new comprehensive synthesis is required because each of the existing documents (see above) contains a part of the story but not all written up at the final point in model development and implementation when everything has to ‘hang together’.

3.2. Knowledge of present-day groundwater salinities and initial state for modelling

Knowledge of the present-day values and distribution of groundwater compositions is necessary because it provides a basis for testing and calibrating the regional-scale model of salinity evolution. That is done by running a model of palaeohydrogeological evolution of salinities from a starting point in the past through to the present day and onwards into the future. Other relevant reasons for knowing groundwater compositions are to develop an understanding of what controls salinities and specific ionic solutes that influence safety functions of the EBS, and to identify the reference waters that are the basis for a mixing model of salinity evolution.

Compositions of pore waters in the rock matrix also need to be known. Pore waters exchange diffusively with groundwaters in fractures and therefore will modify future groundwater salinities, making them more or less saline depending on the relative concentrations. Pore water compositions also are evidence of groundwater compositions in the past, i.e. whether more or less saline than at present, though interpretation in this sense is qualitative and cannot provide detailed information about salinity changes in the past.

SKB has made all reasonable attempts to characterise compositions of groundwaters in deformation zones and fractures and has also analysed chloride in pore waters in drillcores from a few boreholes. The spatial variability of salinities at repository depth is fairly well established. For example, the depth variations of salinity in rock above the target volume vary from dilute to brackish. It is evident that salinities at repository depth in the target volume comprising fracture domain FFM01 are brackish to saline, whereas outside the target volume salinities are lower. Although sampling groundwaters becomes more difficult and data are sparse in less fractured rock and less transmissive fractures, there are sufficient information to be confident about the ranges and distributions of salinity and confident that dilute groundwater does not currently exist anywhere in the target volume.. Groundwaters sampled below 300 m depth all had Cl^- concentrations above about 6000 mg/L and the depth trends for fracture waters and pore waters do not indicate any anomalies.

My assessment is that the level of knowledge of groundwater compositions, their distribution and the sources of the different water components that constitute the present groundwater system is generally adequate as the basis for forecasting likely long-term evolution of salinity.

Monitoring of groundwaters at repository depth during construction and operation of the repository would be necessary, to confirm the spatial variations of salinity in more detail and to detect any indications of diluting effects of groundwater drawdown or conversely of salinity increase due to upconing.

Regarding selection of initial state for the numerical model of salinity evolution, SKB has decided to simulate forwards from an initial state representing groundwater compositions 10,000 years ago. This means that the model is tested and calibrated by comparing modelled and measured present-day compositions. Initial state and present-day compositions are described in terms of salinities and proportions of reference waters.

SKB's choice of an 'altered meteoric' reference water for which the composition already exceeds the >4mM criterion of the safety function indicator $\Sigma q[M^{q+}]$ leads to a rather confusing position in salinity evolution modelling in that using it would not test sensitivity of dilution to hydrogeological influences. SKB has recognized that and has circumvented the issue by doing the key dilution modelling for the temperate period with an end member with zero salinity to test a 'worst case' of infiltrating water composition (the glacial melt reference water is very dilute so does pose this issue). Whilst accepting this as a pragmatic and valid approach to choosing a representative composition for dilute infiltration, I have the impression that this choice by the modellers is rather obscured by discussion about the altered meteoric reference water. This is one of many aspects of the salinity evolution modelling where the report lacks clarity and leaves the reader to work out what was actually done. It leaves the impression that the planning, implementation and reporting of salinity evolution modelling and dilute water penetration were done with a degree of ad hoc expediency. I think that the approach is basically robust and justifiable, but the description of what has been done is tortuous and difficult to follow.

3.3. Probability of dilute water entering deposition holes

The modelled frequency and distribution of deposition hole positions that might experience water more dilute than the $\Sigma q[M^{q+}]$ >4 mM threshold of acceptability depend on two basic outcomes of groundwater modelling: the spatial and temporal development of water dilution, and the movement of diluted water into deposition hole locations where it would come into contact with buffer. The former modelling is done as an equivalent continuous porous medium (ECPM) and is therefore an averaged approximation of how salinity will evolve. Salinity changes are mainly due to changing infiltration compositions, changing hydrodynamics, mixing which is simulated as a result of hydrodynamic dispersion, and diffusive exchange with matrix pore waters. The latter modelling is done as a discrete fracture network (DFN) and is a probabilistic representation of transmissive fractures with properties constrained by selected geometric and parametric relationships. Salinity changes are defined in space and time by what the ECPM model outputs and also by an analytical model for diffusive exchange with pore waters.

The ECPM modelling uses a state-of-the-art numerical code and is well proven in previous stages of SKB's programme as a valid approach to simulating transport and mixing of Cl^-, salinity or proportions of reference waters. SKB states that confidence is high in the DFN model, and that there are greater remaining uncertainties in the properties of the deformation zones (DZs). More transmissive DZs would result in more rapid advance of dilute groundwater. SKB have not, as far as I understand it, shown that salinity evolution through the ECPM regional-scale model is the same as it would be through the site-scale DFN from which the ECPM has been parameterised. Connectivity, anisotropy, channelling and flow-wetted surface area of the ECPM should be reflected in the properties of the ECPM that affect the propagation of water dilution. These aspects of the DFN are outside my expertise and I assume that these will be dealt with in other expert reviews, so in that context I assume that the ECPM-DFN equivalence is adequate for this purpose of salinity evolution and dilute water penetration modelling.

The regional-scale model has been calibrated against pumping test data and also calibrated against observed chemical and isotopic water by palaeohydrogeological modelling from 10,000 years ago to the present day. Vertical hydraulic conductivity was reduced by an order of magnitude to improve the fit to hydrochemical and interference test data. This approach to large-scale flow and transport properties looks as robust as can reasonably be achieved, though its limitations as a simplistic 'curve matching' comparison need to be taken into account in considering potential uncertainties. However calibration has been possible only for the shallower part of the system, above -400 m, because availability of relevant data is less dense towards repository depth. If the lower hydraulic conductivity suggested by calibration for shallower parts of the system also applies at repository depth, it would decrease the calculated rate of dilute water penetration through the DFN. Overall I conclude that there are relatively large remaining uncertainties in the ECPM representation of salinity evolution and the extent of dilute water penetration towards repository depth, although these uncertainties probably mean that the results of the modelling are pessimistic in terms of DFN transmissivity and penetration of dilute water.

The duration for which dilute water invades the system is the key factor in how the ECPM model of salinity evolution develops. Both duration of dilute water invasion and fracture distribution and properties are evidently key factors in how the DFN model for dilute water at deposition hole positions develops.

Simulations of salinity evolution and dilute water infiltration during the temperate period of the base case evolution have mostly been limited to a duration of 10,000 years and the variant scenario with an extended temperate period due to global warming has a duration of 60,000 years. The durations of the base case simulations are rather inconsistent which is confusing – some go to 7,000 or 9,000 years in the future rather than 10,000 years, whilst the hydrogeochemical model simulations go to 7,000 years, but this does not substantially affect the value of the model results.

The reporting of modelling for the extended temperate period is less satisfactory with very little information being provided. It is unclear whether the extended duration model is identical to the 10,000 year model, or whether some changes had to be made to the basic model to run it for the much longer timescale. The very limited graphical illustration of results, just one cumulative distribution plot with a logarithmic timescale, allows only a simplistic comparison between model outputs for the two timescales.

A number of varying scenarios and timescale have been modelled for glacial melt water infiltration including infiltration under fully glaciated conditions for an extended timescale of 100,000 years. Another model variant has assumed glacial conditions for 25% of the 120,000 years duration of the next glacial cycle. These hypothetical scenarios are pessimistic simulations and therefore are adequate assessments of the maximum likely infiltration of dilute water.

Uncertainties in measured pore water salinities have probably been underestimated, but nevertheless it is evident that diffusive exchange between fracture waters and pore waters could be a significant buffer of future salinity evolution in fracture waters. SKB's model for solute exchange between fracture waters and pore waters is simplified by assuming that the entire matrix is accessible by diffusion. The evidence to support this assumption is, in my opinion, scant although the evidence for any such limitation is also absent. If that assumption is invalid, or the values for solute diffusivity of the rock matrix or for flow-wetted surface area of fractures have been overestimated, then matrix exchange will be less effective than modelled at attenuating dilute water advance. The sensitivity of dilute water attenuation to these factors has not been reported in detail, though SKB state that this has been done and that it is not a primary issue.

The value assigned to dispersivity in the ECPM model influences the transport of solutes and therefore the penetration and mixing of dilute water infiltration. Uncertainty in the concept and parameterisation of dispersion means that the degree of dilution at repository depth could be over- or under-estimated. If the value is too high, the model will simulate too much dispersive mixing with pre-existing saline water and excessive attenuation of infiltrating dilute water. SKB could provide more explanation of how hydrodynamic dispersion is represented in the models at different scales and whether or not there is a significant dependence of dilute water mixing and attenuation on the choice of dispersion length.

Regional-scale modelling of salinity evolution through a glacial period has been done by SKB in a very similar way to the temperate period modelling. The initial salinity of groundwaters at repository depth at the end of the temperate period and at the start of a glacial period has been assigned a value of 3 g/L TDS, as also has the salinity of pore waters in the rock matrix. Modelling of salinity through the prolonged temperate period indicates that it would probably be much less than 3 g/L, so the value presumably corresponds to the relatively short temperate period in the reference evolution rather than the global warming duration of 60,000 years. SKB should explain how the model results would be affected by assigning a lower initial salinity.

The very dilute composition of glacial melt water that is assumed as the boundary condition for the evolution of salinity through a glacial period, plus the fact that the salinity evolution model does not include reaction of melt water with rock, means that the regional-scale model is likely to underestimate the increase of mineralisation in glacial melt water during the early stages of infiltration, prior to mixing with pre-existing groundwater components.

SKB presumes that melt water infiltration will occur only over a period of tens to hundreds of years as the edge of an ice sheet might advance or retreat over the site. This is more or less the current paradigm for sub-glacial hydrology, though the evidence to support it is sparse and rather incoherent and it is an area of ongoing research. It is therefore sensible that precautionary ‘worst case’ model calculations of sub-glacial infiltration have been done by SKB and they satisfactorily prove that, at least as far as the dilute composition of melt water and sub-glacial hydraulics are concerned, the safety analysis is robust to the degrees of uncertainties.

Diffusive exchange with pore waters in the DFN models is simplistically simulated with an analytical formula, without any restriction on accessibility of the matrix to exchange. The analytical formula uses the transport resistance (‘F’) for fracture pathways calculated in the DFN. It seems that SKB has not evaluated the sensitivity of the dilute water penetration model to uncertainty and variability in F values. SKB does not offer any expert judgements on this matter. The relationships between the vulnerability of flow paths and deposition holes to dilute water penetration and the magnitudes of calculated F values are shown by SKB to be rather complex. This may be significant because diffusive exchange is the only process that attenuates dilute water. Further investigation and explanation of this would increase confidence that the uncertainties are secondary.

The limited scope of DFN realisations and variants for modelling of dilute water penetration in glacial conditions suggests that, taking a qualitative view of the large uncertainties in virtually all aspects of glacial and sub-glacial processes, the number of deposition holes affected might exceed SKB's deterministic estimate by several times, perhaps up to 500. The key determinant of which deposition holes are 'at risk' of dilute water penetration seems to be the distribution and properties of DFN fractures, but SKB has not provided a convincing argument that the uncertainties in DFN fracture representations are constrained by the presented DFN variants.

In another, pessimistic, illustration of risk, SKB forecasts that only one deposition hole will experience a combination of flow velocity and water dilution of such severity that buffer will be eroded to the point of reaching advective conditions at the canister surface. The assumptions implicit in this estimation, especially the role of water flow velocity in contact with the buffer, have not been explained. It is unclear how this conclusion compares with the other illustrative calculations of 'number of deposition holes receiving dilute water'. However, taking the various illustrations at face value, the probability of buffer erosion by dilute water looks very low. There would be greater confidence that this conclusion is valid if SKB could make a clearer case for the validity of the DFN representation of fracturing and transmissivity around deposition tunnels on which the conclusion seems to be dependent.

My understanding is that HRD bedrock between DFN fractures is assumed by SKB to be unfractured and thus to transmit water only by diffusion. SKB does not provide a complete conceptual description of this 'unfractured' rock that will surround most of the deposition holes, so I am uncertain about whether and how, given sufficient time, dilute water will eventually contact the buffer. Does the 'unfractured' rock contain micro-fractures that transmit water very slowly, above a purely diffusive threshold but below a threshold of advection that would be significant in terms of buffer erosion and radionuclide transport? If the fabric of intact bedrock is below the diffusion threshold, then where does water for resaturation of buffer come from, and what are the implications of that for water composition and flow velocity? I think that these uncertainties will only be resolved by monitoring of experimental or pilot emplacements at the early stages of construction.

Overall, SKB's reporting does not give me a sufficiently high degree of understanding and confidence that the conceptual model for water and solute transport and diffusion in the rock around deposition holes, typically over a distance scale of 10 metres or so, is a conservative representation of all possibilities for behaviour in the actual bedrock system.

However in the context of the present evaluation which concerns dilute water penetration to deposition holes and the consequent risk of chemical erosion of buffer, the uncertainties arising from the DFN treatment of water transmission into deposition holes may be of secondary importance. That is because the mineralisation of groundwater at repository depth, even water that has been diluted due to prolonged infiltration of meteoric or glacial melt water, is very likely to be higher than the $\Sigma q[M^{q+}]>4mM$ criterion for the buffer safety function. The compliant level of mineralisation will have been acquired due to mineral dissolution reactions, mixing with pre-existing brackish/saline groundwaters and diffusive exchange with brackish pore waters.

In summary, my assessment of how SKB have handled salinity evolution is that there are various uncertainties in the ways that solute transport, groundwater mixing and salinity attenuation by matrix diffusion have been modelled and constrained. These uncertainties could potentially cause substantial variability in the patterns of salinity development through time in the bedrock, specifically at repository depth and around deposition hole positions. However, given the specific threshold of <4 mM for dilution to become significant with regard to buffer erosion, my judgement is that it is very unlikely that deposition hole positions would experience such significantly dilute inflows.

For buffer erosion to be of such severity that groundwater advectively transports sulphide corrodant to a canister surface, groundwater inflow through a fracture intersecting a deposition hole must have a relatively high flow rate as well as a very dilute composition. The construction and parameterisation of the hydrogeological DFN model is key to predicting how many deposition hole positions, given successful implementation of the FPC/EFPC (full perimeter intersection criterion) acceptance criteria, would have such high flow rates. In my opinion, SKB’s DFN conceptualisation and testing of variant models and uncertainties is incomplete and poorly reported, and therefore the numbers of deposition holes that could conceivably experience such inflows are more uncertain than so far suggested. Nevertheless, the high level of confidence that ‘dilute’ water compositions will always be compliant with the buffer safety function requirement means that I do not consider those DFN uncertainties in inflow rates to be problematic for buffer stability.

In that respect, I agree with SKB’s conclusion although it has not excluded the possibility of a small number of affected deposition holes. With regard to that pessimistic position, I would just comment that SKB’s model of salinity evolution for this purpose omits the influence of hydrogeochemical reactions in establishing a ‘base level’ of mineralisation, relying just on hydrodynamic mixing and diffusive exchange with pore waters to modify salinity.

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Coverage of SKB reports

Reviewed report	Reviewed sections	Comments
Technical Report TR-11-01. SKB 2011. Long-term safety for the final repository for spent nuclear fuel at Forsmark. Main report of the SR-Site project.	4.6 to 4.9; 6.2; 10.3 to 10.6; 12.2	[*insert comments, if any*]
Report R-09-20. Joyce, S., Simpson, T., Hartley, L., Applegate, D., Hoek, J., Jackson, P., Swan, D., Marsic, N. and Follin, S. 2009. Groundwater flow modelling of periods with temperate climate conditions – Forsmark.	Whole report, primarily Sections 3 to 6 and Appendices C & F	
Report R-09-21. Vidstrand, P., Follin, S. and Zugec, N. 2010. Groundwater flow modelling of periods with periglacial and glacial climate conditions – Forsmark.	Sections 3 to 6; Appendices D to G	
Technical Report TR-10-58. Salas, J., Gimeno, M.J., Auqué, L., Molinero, J., Gómez, J. and Juárez, I. 2010. SR-Site – hydrogeochemical evolution of the Forsmark site.	Sections 3, 4, 6, 7; Appendices 2 & 3	
Report R-08-82. SKB 2008b. Confidence assessment. Site descriptive modelling SDM-Site Forsmark.	Reference only	
Report R-07-49. Follin, S., Johansson, P-O., Hartley, L., Jackson, P., Roberts, D. and Marsic, N. 2007. Hydro-geological conceptual model development and numerical modelling using CONNECT-FLOW, Forsmark modelling	Sections 2, 3, 4, 6	

stage 2.2.	
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Report R-08-95. Follin, S. 2008. Bedrock hydrogeology Forsmark. Site descriptive modelling, SDM-Site Forsmark.	Reference only
Report R-09-22. Selroos, J-O. and Follin, S. 2010. SR-Site groundwater flow modelling methodology, setup and results.	Reference only
Technical Report TR-08-05. SKB 2008a. Site description of Forsmark at completion of the site investigation phase. SDM-Site Forsmark.	Reference only
Technical Report TR-10-52. SKB 2010a. Data report for the safety assessment SR-Site	Section 6 (Geosphere Data), primarily 6.7 & 6.8 (Migration properties)
Technical Report TR-10-54. SKB 2010b. Comparative analysis of safety related site characteristics.	Reference only
Report R-08-105. Waber, H.N., Gimmi, T. and Smellie, J.A.T. 2008. Porewater in the rock matrix. Site descriptive modelling SDM-Site Forsmark.	Reference only

2014:47

The Swedish Radiation Safety Authority has a comprehensive responsibility to ensure that society is safe from the effects of radiation. The Authority works to achieve radiation safety in a number of areas: nuclear power, medical care as well as commercial products and services. The Authority also works to achieve protection from natural radiation and to increase the level of radiation safety internationally.

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