Strål
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Swedish Radiation Safety Authority

2016:08

SSM's external experts' reviews of SKB's safety assessment SR-PSU – hydrogeological and chemical aspects

Initial review phase

Report number: 2016:08 **ISSN:** 2000-0456
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SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) received an application for the expansion of SKB's final repository for low and intermediate level waste at Forsmark (SFR) on the 19 December 2014. SSM is tasked with the review of the application and will issue a statement to the government who will decide on the matter. An important part of the application is SKB's assessment of the long-term safety of the repository, which is documented in the safety analysis named SR-PSU.

Present report compiles results from SSM's external experts' reviews of SR-PSU. The general objective of these reviews has been to give support to SSM's assessment of the license application. More specifically, the instructions to the external experts have been to make a broad assessment of the quality of the application within the different disciplines and to suggest needs for complementary information. The results may also be helpful in guiding SSM to detailed review issues that should be addressed in the assessment of the application.

Table of Contents

Project information

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Contact persons and registration numbers for the different expert review contributions are given in the report.

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Review of hydrogeological site-descriptive model SDM-PSU – 1

Activity number: 3030014-1001
Registration number: SSM2015-1016
Contact person at SSM: Georg Lindgren

Abstract

The Swedish Nuclear Fuel and Waste Management Co. (SKB) has proposed to extend the SFR facility for low- and intermediate-level radioactive waste, located near Forsmark, Sweden. In support this proposal, SKB has presented a site descriptive model, SDM-PSU. This report presents findings of an initial-phase review of hydrogeological aspects of SDM-PSU, considering the relevance for SKB's safety assessment SR-PSU. Hydrogeological models are utilized directly in SR-PSU for calculating flows through the waste vaults and paths for radionuclide transport.

The documentation of hydrogeological aspects of SDM-PSU is well structured and sufficiently transparent for review. Assumptions and methods are generally well explained, and detailed appendices provide traceability regarding the use of data. Handling of uncertainties, particularly between the background reports and the main SDM-PSU report, is less clear.

The scientific approach is credible but the resulting model is not fully mature as a basis for safety assessment in support of a license application. Use of older data from the existing SFR is incomplete; the explanations given for discrepancies are not sufficient to give confidence in a model that does not use the older data. Possible lateral trends in hydraulic properties are not explored to the same extent as vertical trends. Practically no data support extension of the rock-mass hydrogeological model to the northern boundary belt. Treatment of stochastic uncertainties for the rock mass is very limited. A stochastic model of the inferred “shallow bedrock aquifer” is illustrative but non-systematic.

Multiple hypotheses are proposed to explain time-dependent declines in inflows to the existing SFR vaults and tunnels, but little evidence is presented for their quantitative impact. Hypotheses for “skin effects” both at the marine sediment/bedrock interface and in tunnels appear to be important for calibration of the models, but have not been tested. The important hypothesis of a compartmentalized system has not been tested by use of packer-test data as a complement to difference flow logging data.

Recommendations are given for clarification and independent review of these issues.

Contents

1. SKB's Presentation

Since 1987 the Swedish Nuclear Fuel and Waste Management Co. (SKB) has operated an underground repository for low- and intermediate-level radioactive waste, the SFR, at a location near Forsmark, Sweden. In support of a proposed extension of this facility, SKB has presented a site descriptive model, SDM-PSU which encompasses the bedrock volume hosting the existing SFR as well as the proposed extension (Figure 1).

This summary of SKB's presentation of hydrogeological aspects of SDM-PSU is divided into two main areas: A summary of the relevant documentation, and a discussion of the safety relevance of the review area. These two areas are covered in successive sections of this chapter.

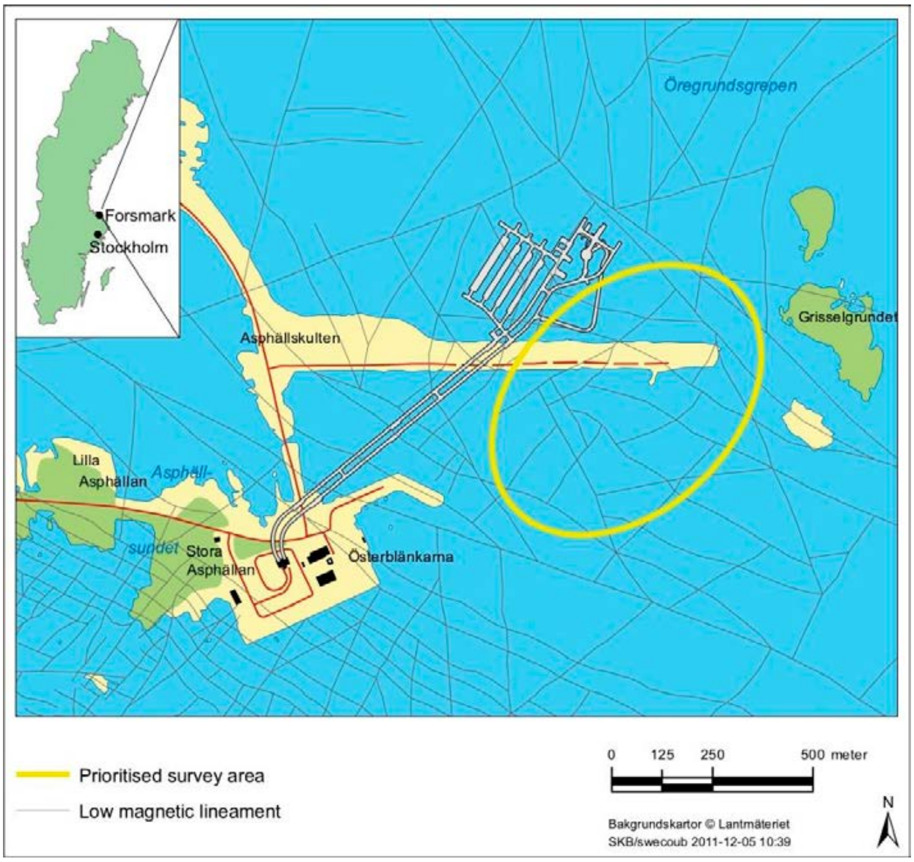

Figure 1: Map of the Forsmark-SFR area showing the location of the existing SFR and the area that was prioritized for an extension of this facility. From Figure 1-1 of SKB-R-11-10.

1.1. Relevant documentation

The documentation considered in this review begins with the top-level report that describes the site-descriptive model SDM-PSU, and the main hydrogeological background reports, which together provide an overview of the hydrogeological investigations and site-descriptive model development. Other reports considered here cover planning of the site investigations, data acquisition and interpretation, modelling and application to SR-PSU. These are discussed in sequence in the following subsections.

1.1.1. Top-level documents

The SDM-PSU main report (SKB TR-11-04) gives a top-level description of the geoscientific site investigations, analyses, and synthesis leading to the site-descriptive model for SR-PSU.

The main sections of interest for hydrogeological review are:

- Chapter 2 which describes the investigations that were carried out from the surface, tunnels within the SFR facility, and boreholes, and
- Chapter 7 which describes the bedrock hydrogeology.

The latter chapter is essentially an abbreviated version of the bedrock hydrogeology report (Öhman et al., 2012, SKB R-11-03) plus a summary of the groundwater flow modelling report for the SFR site investigation (Öhman et al., 2013, SKB R-11-10). Chapters 2, 4, 5, and 6 of SKB R-11-03 correspond closely to Sections 7.1 through 7.4 of the SDM-PSU main report, but give further detail. The description of groundwater flow modelling in Section 7.5 of the main report is a very condensed summary of SKB-11-10. The discussion of confidence and remaining uncertainties in the main report draws on these two supporting reports, but is substantially restructured and rewritten.

Several other parts of the SDM-PSU main report are relevant for hydrogeological review, as discussed in the following paragraphs.

Evolutionary aspects of groundwater at the site are discussed Section 3.4. Characterization of the regolith is described in Section 4.1.2 (though the regolith depth & stratigraphy model used in SR-PSU is updated from SDM –PSU, making use of additional depth and stratigraphy data from probing and drilling in wetlands).

Meteorology, hydrology and near-surface hydrology are discussed very briefly in SKB TR-11-04 Section 4.1.3, which refers to modelling studies by Bosson et al. (2008) and Mårtensson and Gustafsson (2010), and Mårtensson et al. (2010) that were carried out for the spent-fuel repository license application, for further information.

A brief section on coastal oceanography (SKB TR-11-04 Section 4.1.4) covers the definition of marine sub-basins, but does not discuss sea level fluctuations (e.g. due to Baltic storm events) which could potentially influence groundwater flow and solute dispersion in the shallow bedrock. A more detailed treatment of time-dependent sea levels is included in the modelling for SR-PSU (Werner et al., 2013).

Hydrogeochemistry of the surface system is discussed briefly in TR-11-04 Section 4.1.5. Surface-bedrock interactions are discussed very briefly in TR-11-04, Section 4.4, referring to conceptual model development and calculations that were conducted for SR-Site (Olofsson et al., 2007; Follin, 2008; Bosson et al., 2010; Johansson, 2008).

Geology as presented in Chapter 5 of SKB TR-11-04 is pertinent for information on the large-scale and small scale structures that pertain to the hydrogeological conceptual model in terms of Hydraulic Conductor Domains (HCDs) and discrete-fracture network (DFN) models of the Hydraulic Rock Domain (HRD), respectively. Laboratory measurements of hydraulic normal fracture stiffness described in Section 6.2.2 of SKB TR-11-04 may be relevant for coupled stress-flow modelling.

1.1.2. Site investigation planning

The main planning document considered in this review is SKB R-08-67 (SKB, 2008, in Swedish). The main chapter for hydrogeological issues is Chapter 7. The introductory section states the goals of the hydrogeological investigations, and the central questions that these investigations were aimed to answer:

- Extent and hydraulic properties of gently dipping, unloading joints and/or deformation zones within the prioritized rock volume;
- Hydraulic properties of the interpreted low-magnetic lineaments;
- Rock mass hydraulic properties within the prioritized area and the variability of properties depending on differences in rock type;
- Scale and characteristics of hydraulic connections with the prioritized area as well as between these and the surrounding rock.

The hydrogeological investigation methods that were planned to be used in different boreholes are laid out in Section 7.3 of this report, along with brief explanations and references to SKB's method descriptions for each of the borehole hydraulic measurement methods used, and instructions for analysis of injection and single-hole pumping tests.

Section 9.2.3 of SKB R-08-67 gives a concise summary of previous hydrogeological data evaluations and mathematical modelling that were carried out in connection with the construction and operation of the SFR facility, and which form the basis for SDM v.0. A brief summary is also given of the main conclusions from modelling by Holmén and Stigsson (2001a, 2001b). Section 9.3.3 gives a very brief summary of plans for further development based on the hydrogeological investigation methodology laid out by Rhén et al. (2003).

1.1.3. Model domains

Two different model scales are used for site descriptive modelling of bedrock geology in SDM-PSU: a local scale that covers an 860 m x 720 m area immediately around the existing SFR and the proposed expanded facility, extending to 300 m below present-day mean sea level, and a regional scale that covers a 1550 m x 1685 m area surrounding the local-scale volume (Figure 2) and extending to 1100 m below sea level. Both of these volumes are stated to extend up to 100 m above present-day mean sea level. However as seen from Figure 2, only a small part of the area within the either the local area or the regional area is above sea level (a few islets of low topographic relief and several rock causeways and jetties, with a maximum elevation about 6 m above sea level).

A larger hydrogeological model area was used for hydrogeological modelling for SDM-SFR, defined in terms of surface water divides (Figure 3).

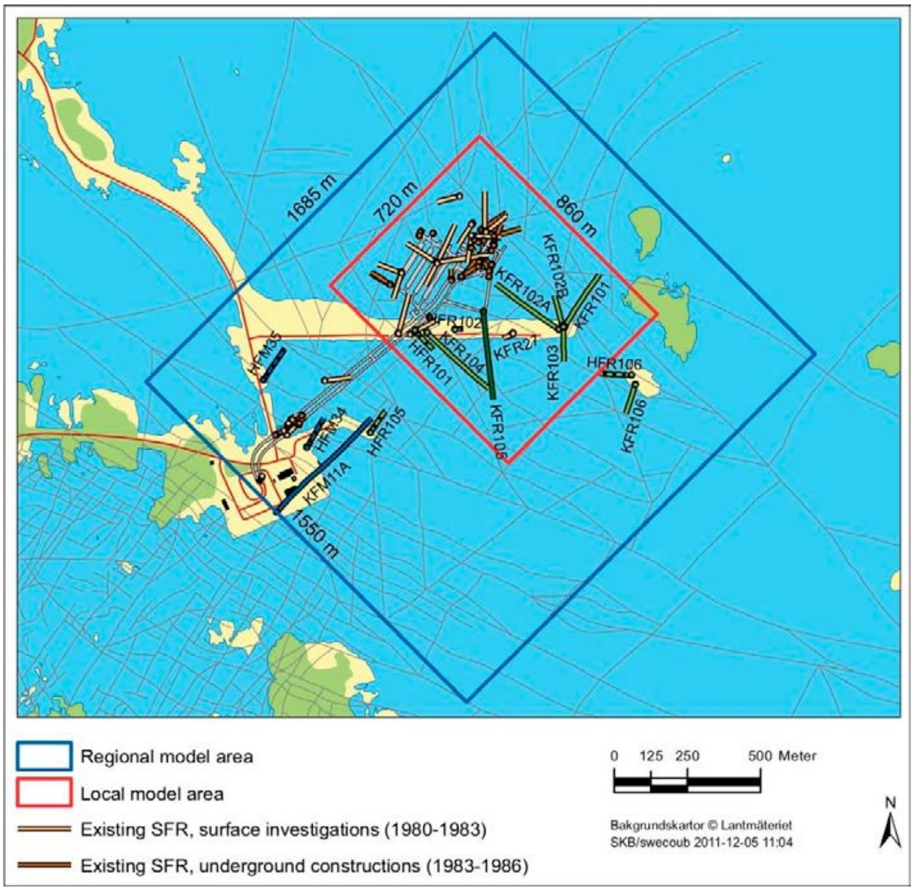

Figure 2: Local and regional model areas for SDM-SFR, showing borehole coverage for different stages of investigation (according to the color key for investigations related to the existing SFR, and different shades of green for more recent stages of investigations for the SFR extension). From Figure 1-2 of SKB-R-11-10.

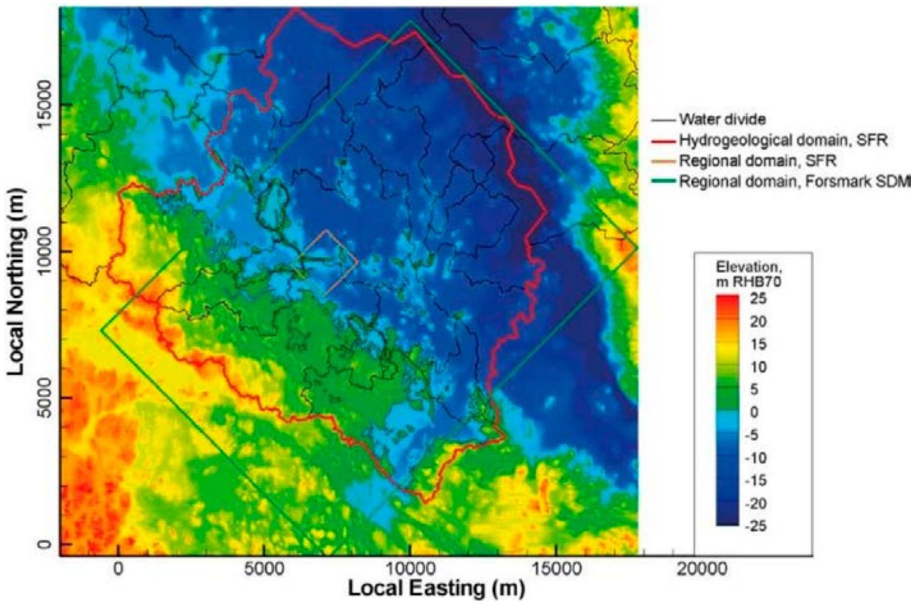

Figure 3: Hydrogeological domain used for SFR hydrogeological modelling (irregular area outlined in red, along surface-water divides), in relation to the regional domain for the bedrock site-descriptive modeling in SDM-SFR (orange rectangle) and the regional domain for hydrogeological modelling in site-descriptive modelling for the proposed spent-fuel repository at Forsmark (green rectangle). The local coordinate system has its origin with respect to the national (RT) coordinate system at RT Northing = 6,692,000, RT Easting = 1,626,000. From Figure 1-3 of SKB-R-11-10.

1.1.4. Data acquisition and interpretation

The SDM bedrock hydrogeology report (Öhman et al., 2012, Table 1-4) includes a list of data that were used, with reference to specific sources whether in SKB's Sicada database, tables in published reports, RVS or GIS models, or other specific SKB documents. More detailed account of specific datasets and their use in the analysis are given in the chapter on evaluation of primary data (Chapter 4) and in the appendices, particularly Appendices D through H which detail (D) a re-analysis of hydraulic data from the construction of the SFR, (E) analysis of hydraulic data from the extension of the SFR, (F) monitoring data of head and sea level fluctuations, (G) DFN analysis, and (H) characterisation of shallow-bedrock-aquifer structures (SBA).

Key supporting references include SKB P-04-49 (Öhman and Follin, 2010) and SKB P-10-43 (Walger et al., 2010).

Öhman and Follin (2010) give a detailed account of the interpretation of hydraulic data in terms of parameterizations for the HCDs and HRDs. The analysis is used to justify models for trends in hydraulic properties of these domains with depth, as developed further by Öhman et al. (2012).

Walger et al. (2010) give evaluations of the pressure responses in all instrumented SFR-boreholes, in response to hydraulic perturbations due to four interference tests and due to the drilling of six boreholes (one of the four interference tests, in the shallow percussion-drilled borehole HFR102, produced no identifiable responses).

1.1.5. Conceptual model and parameterization

The conceptual hydrogeological model proposed by Öhman et al. (2012) is illustrated schematically in Figure 4. The main components as discussed in Section 5.5 of Öhman et al. (2012) are:

- A sparsely fractured Central block described in terms of a discrete fracture network;
- Hydraulic conductor domains (HCDs) of relatively fractured, transmissive rock within this block;
- Southern and Northern boundary belts of relatively intensively fractured rock that provide vertical connections to the seabed and act as positive hydraulic boundaries for the fracture network in the Central block;
- Shallow bedrock aquifer (SBA) structures (mainly sub-horizontal) providing lateral connects in the shallow bedrock;
- Unresolved "possible deformation zones" (PDZs) which are typically subhorizontal, and are treated as part of the stochastic fracture network model;
- Sediments between the seafloor and the bedrock (HSD), with vertical flow constrained both by anisotropy and convergence of flow into bedrock fractures;
- Groundwater flow crossing the inland boundary of this system mainly via an inland shallow bedrock aquifer (described in SDM-Site).

The conceptualization of the discrete fracture network relies on the hypothesis that flow is compartmentalized by "hydraulic chokes" which result from low-transmissivity connections between more well-connected portions of the network.

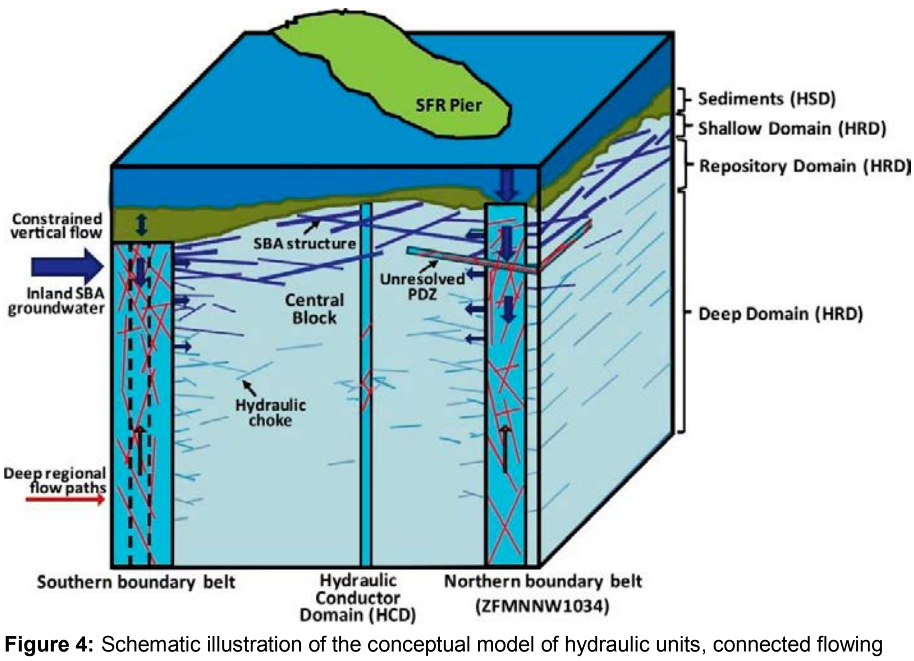

Figure 4: Schematic illustration of the conceptual model of hydraulic units, connected flowing fracture network, and flow paths toward the Central block as proposed and developed by Öhman et al. (2012). From SKB-R-11-03 Figure 5-15.

According to Öhman et al. (2012, p. 101), evidence for a compartmentalized system includes pockets of relict glacial meltwater and Littorina components, the observation of declining flows into the SFR, apparent excess heads that could be explained by land uplift, and low hydraulic diffusivities measured in interference tests.

Hydraulic conductor domain (HCD) parameterization

The parameterization of the HCD structures is developed based on an analysis of transmissivity data for different interpreted HCDs and as a function of depth, as described in Section 5.2.3 and summarized in Section 6.2 of Öhman et al. (2012). The parameters recommended for SDM-SFR are summarized in Table 6-1 of the same report. For the 20 HCDs (out of 40 total) for which no borehole transmissivity measurements data could be assigned, transmissivities and depth trends were assumed based on pooled averages of transmissivity data for HCDs with similar strikes. For most of these, the pooled averages were based just on the newer data from site investigations for the proposed SFR extension, excluding older data (which tended to give higher transmissivities but which were questioned in terms of data quality and geological uncertainties according to Öhman et al., 2012, p. 107).

Hydraulic rock domain (HRD) parameterization

The parameterization of the HRD is based on a discrete-fracture network (DFN) description for three different depth domains:

- Shallow domain (0 to -60 m RHB 70);
- Repository domain (-60 m to-200 m RHB 70) and
- Deep domain (below -200 m RHB 70).

Öhman et al. (2012, p. 109) note that the boundary between the repository and deep domains "may be re-considered once the depth of the SFR extension has been decided." Statistical models for these three domains are presented in tabular form (Öhman et al., 2012, Table 6-2). Two alternative size models are developed, one based on a connectivity analysis and the other on a tectonic continuum assumption.

Deterministic shallow bedrock aquifer (SBA) structures

Six subhorizontal structures, SBA1 to SBA 6 are defined by Öhman et al. (2012) based on hydrogeological data, and a seventh, SBA7, is defined as a possible subhorizontal stress relief structure based on two earlier interpreted horizontal zones (H1 and H3 in the older nomenclature), as shown in Figure 5. An eighth structure referred to as SBA8 is judged to be highly uncertain, although this structure was associated with borehole transmissivities in excess of 10^{-5} m^2/s and required high quantities of grouting.

Öhman et al. (2012, p. 112) regard each of these structures as likely consisting of a network of connected subhorizontal fractures, rather than a single fracture. They also note that the extensions of these structures outside of the area characterized by borehole intercepts are unknown.

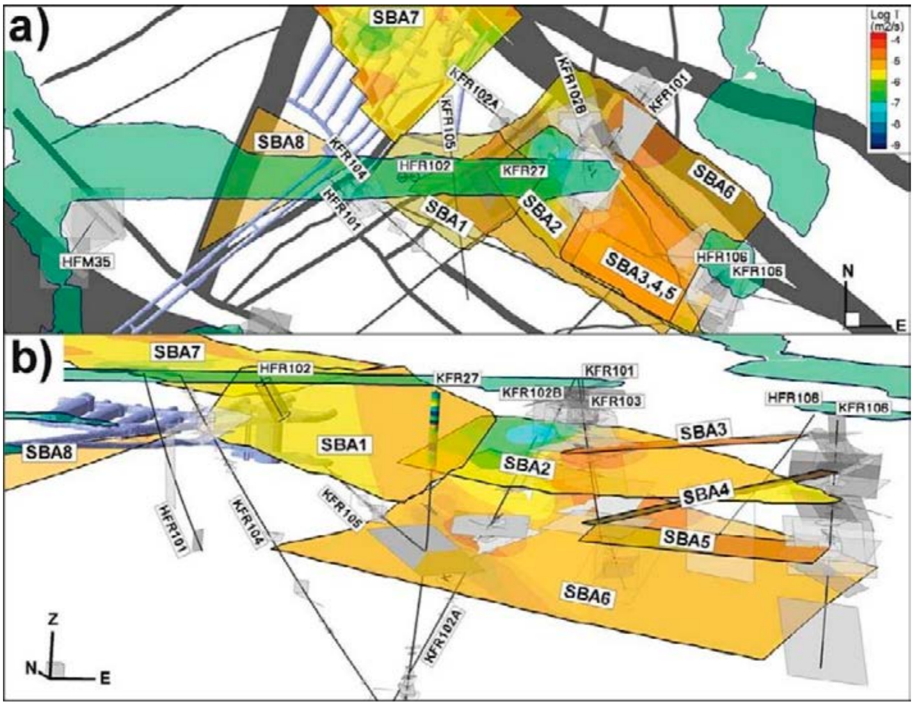

Figure 5: Deterministically modelled shallow bedrock aquifer (SBA) structures (a) top view and (b) side view from the southwest. The structures are coloured by transmissivity according to the scale, as interpreted from the transmissivities at borehole intercepts. The intercepting boreholes are also shown. From SKB-R-11-03 Figure 6-3.

1.1.6. Numerical modelling

A very brief description of groundwater flow modelling for SDM-PSU is given in Section 7.5 of the main report. The main presentation is given in SKB-R-11-10 (Öhman et al, 2013). Additional hydrogeological modelling was carried out, based on an updated model for surface hydrology and the SDM-PSU bedrock hydrogeology model. These models have been addressed in the companion review (Geier, 2015) and the descriptions are recounted in the paragraphs that follow.

Hydrogeological modelling within SDM-PSU

The main presentation of hydrogeological modelling within SDM-PSU is given in SKB-R-11-10 (Öhman et al, 2013). This report recounts the parameterization of hydraulic domains that is described in further detail by Öhman and Follin (2010), and then proceeds with two sets of model exercises:

- Calculations using an equivalent continuum porous medium (ECPM) representation to test the constraining power of borehole data and the effect of different conceptual assumptions on tunnel inflows; and
- Calculations using a discrete-feature representation to simulate the transient response of the interpreted network of HCDs to a series of pumping/interference tests in boreholes.

The ECPM model exercises (described mainly in Chapter 5 of SKB R-11-10) make use of the DarcyTools code (Svensson and Ferry, 2010; Svensson et al., 2010). The discrete-feature model exercises (described mainly in Chapter 5 of SKB R-11-10) make use of the FracMan code (Dershowitz et al., 1998).

The ECPM model exercises using DarcyTools are structured as a series of calculations with increasing model complexity as summarized in Table 5-1 of SKB-R-11-10, starting with a simple homogeneous model of the bedrock (using the uniform, isotropic hydraulic conductivity for the HRD), then considering different degrees of horizontal vs. vertical anisotropy in combination with an HSD.

The HCD structures are then added to the model, initially using calculated properties without conditioning, but then conditioning on values of transmissivity measured at borehole and tunnel intercepts, and imposing a reduced-transmissivity "tunnel skin" around the intersections of HCD structures with tunnels. Two different variants of this model are tested in combination with deterministic SBA structures. A variety of refinements involving connectivity of two specific zones, a depth trend in the HRD, and a supposed "choking" effect of the sediment-fracture interface as well as global moderate anisotropy are also tested. After further adjustments (referred to as "optimization") finally the resulting model is tested in combination with additional, stochastic SBA in the areas outside of borehole coverage.

In Chapter 7 of SKB R-11-10, a different variant of the model, also implemented in DarcyTools and incorporating equivalent continuum porous medium (ECPM) properties for the HRD based on a single realization of a DFN representation, is used to calculate and visualize flow paths for two different flow situations:

- Inflow to the existing SFR (with nominally radial flow to the open repository)
- Topographically driven flow through a hypothetically closed situation for the existing repository.

The results of the latter are used to identify discharge areas for water passing through the existing repository layout.

Discrete-feature model calculations, described in Chapter 6 of SKB R-11-10, are carried out using the FracMan code (Dershowitz et al., 1998) to simulate the transient response of the interpreted network of HCDs to a series of pumping/interference tests in boreholes. The model setup for these calculations does not include the HRD, but just the main HCDs. The calculations are used to compare the interpreted parameterization of the HCDs with the observed hydraulic responses, constrained to propagate via the network of HCDs.

The HCDs are modelled as discrete, quasi-planar structures that are hydraulically connected only via their intersections (Figure 6). SBA structures are also included (Figure 7), and a band of reduced transmissivity at the top of each HCD is used to represent the effect of the HSD in restricting flow from the seafloor.

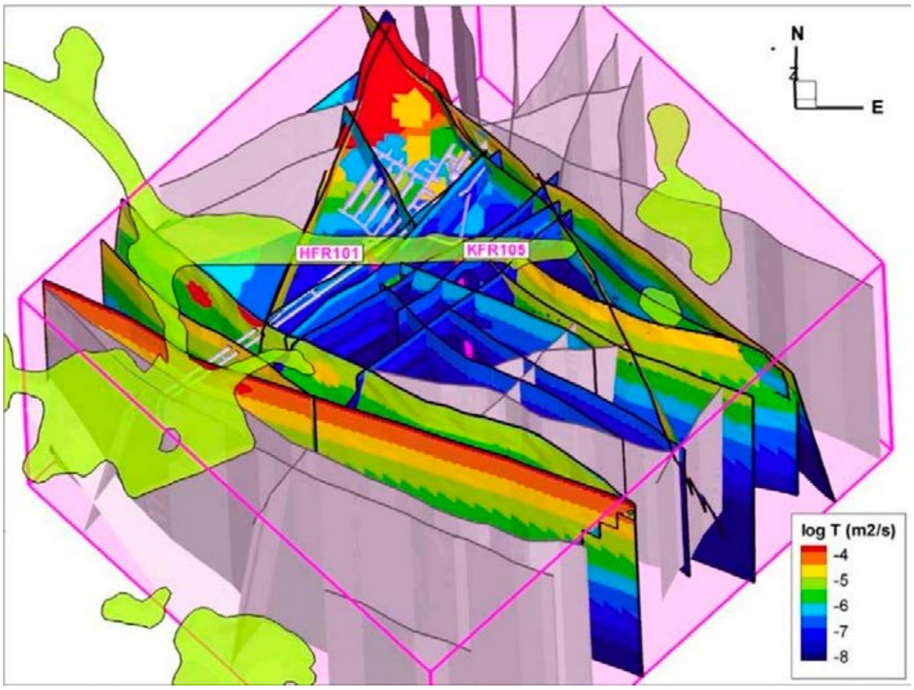

Figure 6: Deformation zones included in the discrete-feature model setup for simulation of interference tests, coloured by transmissivity. Excluded deformation zones are shown in gray. Boreholes where interference tests were performed are shown as pink cylinders. The ground surface is shown in pale green. From Figure 6-13 of SKB-R-11-10.

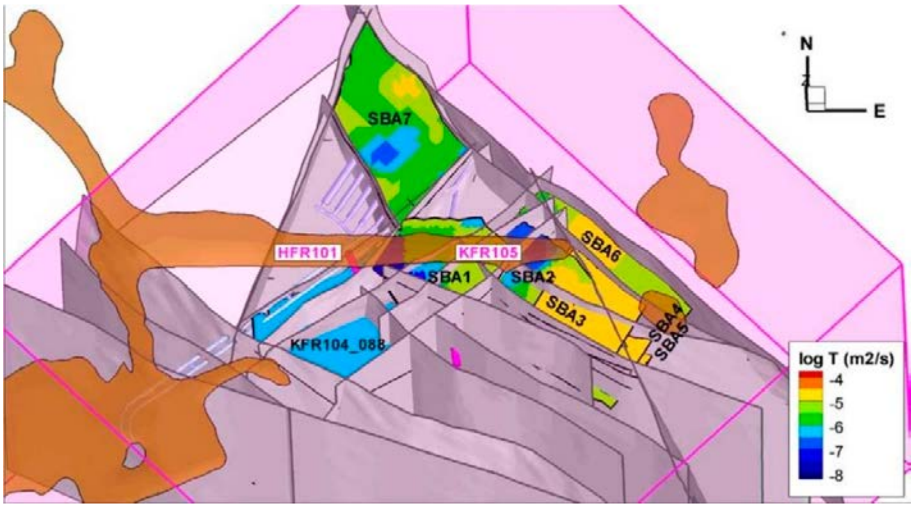

Figure 7: Sub-horizontal structures (SBA1-SBA7 and KFR_088) included in the discrete-feature model setup for simulation of interference tests, coloured by transmissivity. Deformation zones are shown in gray. Boreholes where interference tests were performed are shown as pink cylinders. The ground surface is shown in transparent brown. From Figure 6-14 of SKB-R-11-10.

Within each structure representing an HCD, a zone of reduced transmissivity is used to represent the hypothesized skin effect around tunnels. Another zone of reduced transmissivity is used at the top of each HCD, to represent the hypothesis of a constrained contact between the HSD and the HCD (Figure 8).

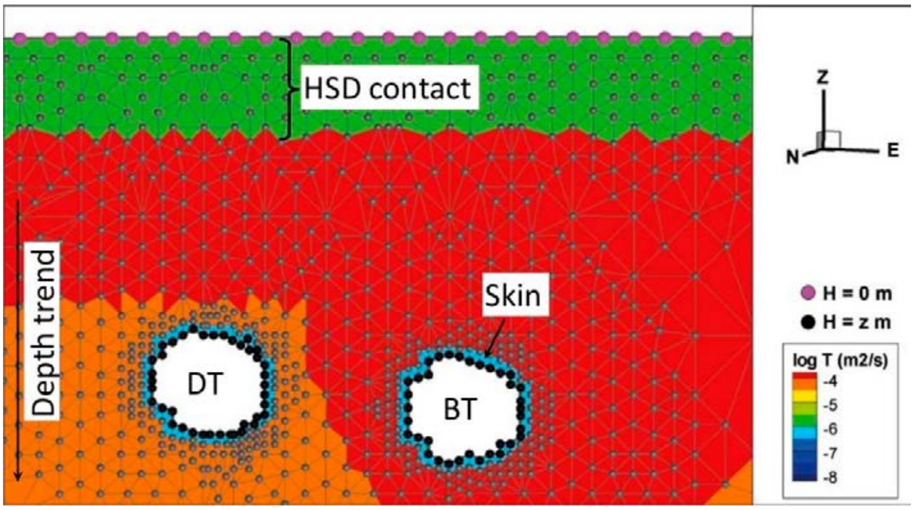

Figure 8: Example of numerical model setup for part of a deformation zone (ZFMWNW0001), illustrating how the hypothesized skin effect around tunnels and constrained contact between the HSD and HCD are represented by zones of reduced transmissivity (as indicated by the color scale). The finite-element mesh is composed of linear triangular elements, with internal nodes indicated by blue dots. The upper boundary condition of prescribed head H = 0 at the seafloor is indicated by the magenta dots. The prescribed atmospheric head at the tunnel walls (*H* = *z*, note that *z* is negative) is indicated by the black dots on the perimeter of the tunnels. From Figure 6-15 of SKB-R-11-10.

Storativity values are assigned based on an empirical relationship to transmissivity:

$$S = 0.0007\,\sqrt{T}$$

as suggested by Rhén et al. (1997), where T is in units of m^2/s (R-11-10, p. 68).

Simulated transient responses for interference tests with pumping in HFR101 and KFR105, are presented graphically and compared in terms of measured response time and peak drawdown values.

Surface hydrology and shallow hydrogeology

R-13-19 (Werner et al. 2013) provides modelling results and descriptions of present and future hydrological and near-surface hydrogeological conditions at Forsmark. The modelling is performed using the MIKE SHE software, as for the equivalent modelling in SR-Site. Results are presented for both present-day temperate and future permafrost/periglacial conditions in terms of water balance, vertical hydraulic head differences between the regolith and the bedrock, depth to the groundwater table, depth of overland water and stream discharge, residence times and inter-basin water exchanges of marine basins. The results for different discharge locations are related to biosphere objects.

Chapter 6 of SKB R-13-19 considers water resources management and exploitation by future inhabitants of the Forsmark area, considering the potential water supplies and capture zones of potential wells, including wells in bedrock. Particle tracking making use of the DarcyTools code is used to investigate the potential for flow to a well to draw in contaminated water for an exposed group farming or growing vegetables in the area. Probability of intrusion of a well is also considered. Thus this report deals with human intrusion issues as well as predictions for the main scenarios.

Far-field hydrogeological modelling for SR-PSU

The hydrogeological modelling for SR-PSU is described by Odén et al (2014; SKB TR-13-25), as a top-level report. Further details of the calculations are given in three progress reports: SKB P-14-04, P-14-05, and P-14-06, as described in the following paragraphs (note these have also been discussed in the companion review by Geier, 2015 and the same summaries are given here).

SKB P-14-04 (Öhman et al., 2014) covers the main hydrogeological calculations for the temperate periods. It assesses of the combined effects of bedrock heterogeneity, parameterisation uncertainty, and transient flow regime in terms of performance measures. A sensitivity analysis is carried out based considering 17 “Bedrock” cases (different hydraulic parameterisations of the bedrock) in combination with six selected stages of shoreline retreat. The main results are in terms of quantitative performance measures for SR-PSU:

- Disposal-room cross flow, Q (m^3/s),
- Coordinates of particle exit locations at the bedrock/regolith interface,
- Flow-related transport resistance along bedrock flow paths, F_r (y/m), and
- Advective travel times along bedrock flow paths, $t_{w,r}$ (y).

SKB P-14-05 (Öhman and Vidstrand, 2014) focuses on interactions between the SFR facilities and potential future water-supply wells in the area. Water-supply wells are considered both for settlements associated with areas that are predicted to have arable land after shoreline retreat according to Werner et al. (2013), and for the “well-interaction area” which has the highest concentrations of radionuclides originating from the repository based on particle-tracking results for the temperate period. The analyses consider both the effect of the wells on flows through the waste vaults in the SFR, and the fraction of well discharge that is drawn from the repository. Wells in the future arable areas are indicated to have very little interaction with flows through the repository. The results for wells in the “well-interaction area” are used in the assessment of the downstream wells scenario.

SKB P-14-06 (Vidstrand et al., 2014) describes hydrogeological calculations for future periglacial periods. The model uses the same bedrock model as for the temperate case, but with thermally/hydraulically coupled solutions for flow and heat transport. Similar to the temperate model, the main results are in terms of quantitative performance measures for SR-PSU:

- Disposal-room through-flows (total and local values),
- Exit locations for particle traces passing through repository vaults an through the bedrock to the bedrock/regolith interface, and
- Darcy fluxes, flow-related transport resistance, path lengths and travel times along bedrock flow paths

The pressure field in the near-field of the SFR is also calculated as input to the near-field flow modelling. Permafrost is studied by means of two variants: One in which the frozen ground reaches elevations just above SFR 1, and one in which frozen ground reaches elevations between SFR 1 and the SFR 3. Results are delivered for combinations of three different bedrock cases, three different permafrost depths, and three different landscape variants.

1.1.7. Application to SR-PSU

The application of the SDM-PSU bedrock hydrogeological model in SR-PSU has two major aspects:

- Demonstration of site understanding
- Quantitative use of modelling results to support safety assessment calculations of radionuclide transport, dose, and risk.

The quantitative links to safety assessment are summarized in in SKB TR-14-09, which is treated in Section 1.2.6 of the companion review (Geier, 2015). The demonstration of site understanding is mainly expressed in terms of the integrated conceptual model with links to hydrogeochemical interpretations, as given in Section 9.7.2 of the SDM-PSU main report. Measured inflows to the existing SFR are also presented but are subject to uncertainties in interpretation as discussed in Section 9.7.3 of the same report.

1.2. Safety relevance of review area

A detailed discussion of the safety relevance of the hydrogeological and surface hydrological issues is given in a separate review (Geier, 2015). A brief synopsis is given here.

The SR-PSU main report (SKB, 2014a) provides a basis for assessing the safety relevance of hydrogeological analysis, presenting a main scenario which is treated as the central case for the evaluating safety, and by comparing the results of the following hydrogeology-related scenarios with the main scenario:

- High flow in bedrock,
- Wells downstream of the repository (Section 7.6.7),
- Intrusion wells (Section 7.6.8),

In addition the following scenarios consider situations where flows through one or more of the vaults can be enhanced by events or processes that lead to omission, breach or degradation of the engineered barriers:

- Accelerated concrete degradation (Section 7.6.3),
- Combination of accelerated concrete degradation with high flow in bedrock (Section 7.8),
- Bentonite degradation (Section 7.6.4),
- Earthquake (Section 7.6.5),
- Loss of barrier function – high water flow in repository (Section 7.7.3),
- Unclosed repository (Section 7.7.6),
- Future human actions (Section 7.7.7)

Figure 9 provides an overview of the relative consequences of these and other scenarios considered in SR-PSU, in terms of the peak annual effective dose.

Hydrogeological aspects of these scenarios, and their impacts on safety according to SKB's evaluation, are summarized very briefly in the subsections that follow.

In addition to these direct ways in which the hydrogeological site-descriptive model and associated uncertainties factor into the risk assessment, another important outcome is in terms of site understanding. Site understanding as reflected in the site-descriptive model does not factor directly into the assessment of risk in SR-PSU, but is important for the credibility of the results and assessment of uncertainty.

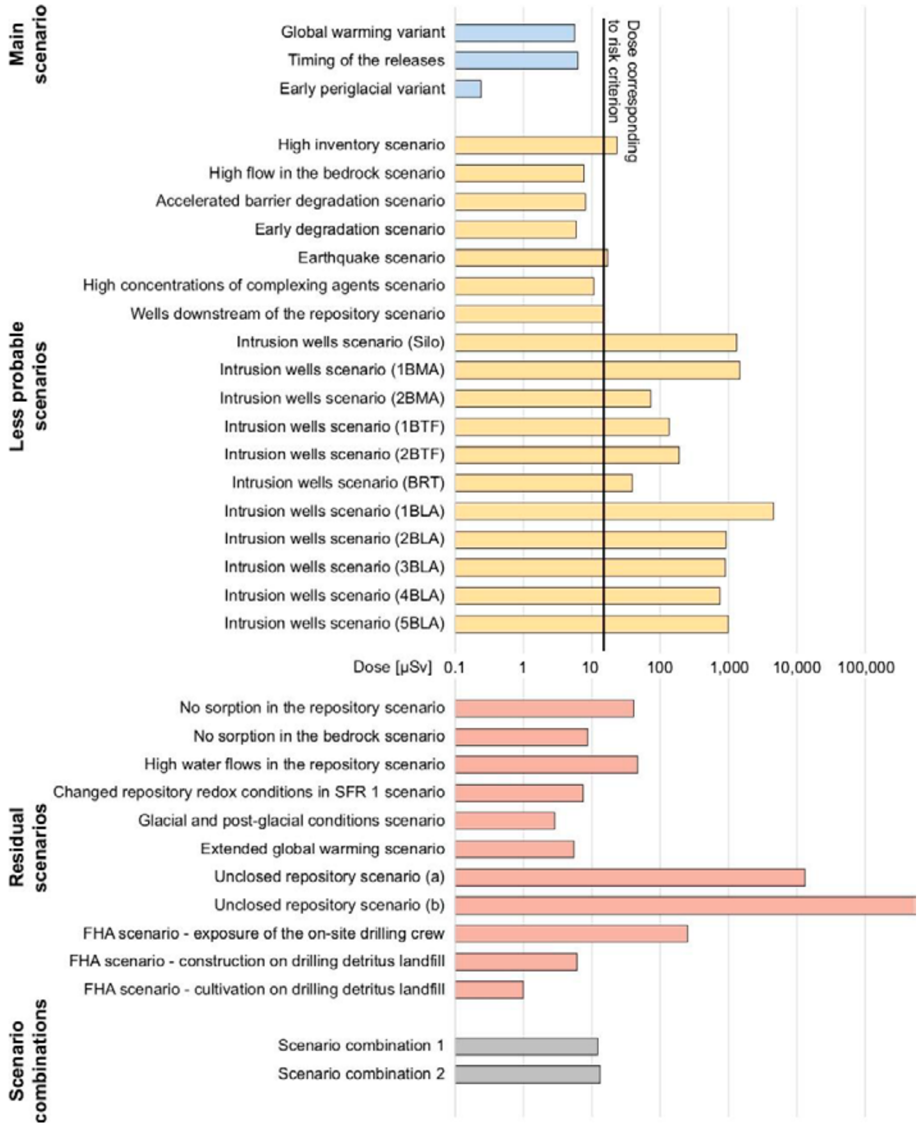

Figure 9: Comparative consequences of the various scenarios modelled in SR-PSU, in terms of the peak annual effective dose (from SKB 2014a, Figure 9-48).

1.2.1. High flow in bedrock

This scenario (Main report, Section 7.6.2) uses hydrogeological data from a bedrock realization (bedrock case 11) that gives high flows relative to the realization (bedrock case 1) that was used for calculations in the main scenario. The outcome (Main report, Section 9.3.2) indicates that it produces a modest, but significant increase in dose especially in the time interval from 3000 to 20,000 AD (Main Report, Figure 9-17). The calculated doses are not sufficient to exceed the risk criterion, but they approach within about a factor of two.

1.2.2. Wells downstream of the repository

The downstream-wells scenario considers the possibility that future human inhabitants could drill wells downstream of the repository after the Baltic shoreline retreats beyond the repository footprint, and that these future inhabitants would then utilize water from these wells for domestic purposes. The assumptions of the scenario are explained in Section 7.6.7 of the Main report.

The results for this scenario are presented in Section 9.3.7 of the main report. For one category of exposed group (a garden plot household), the total dose comes close to this risk-equivalent dose from around 3500 AD to 5000 AD, at which point the risk criterion is briefly exceeded. For other types of exposed groups the dose remains well under the level that corresponds to the risk criterion.

According to the calculation of annual risk in Section 10.3.2, this scenario when added to the main scenario gives the highest maximum annual risk of any of the "less probable" scenarios.

1.2.3. Intrusion wells

The *intrusion wells* scenario is described in Section 7.6.8 of the Main Report. This considers the possibility of a well for drinking water supply being drilled directly into the repository, sometime after the Baltic shoreline has retreated beyond the repository (3000 AD). The probability of such a well penetrating a given vault is estimated based on the current density of wells in the Forsmark area that reach the depth of the given waste vault.

The results as given in Section 9.3.8 of the Main Report show that for a garden-plot household, the annual dose resulting from using drinking water from such a well would exceed the dose corresponding to the risk criterion, for any of the vaults in the early period after 3000 AD, and for most vaults at least until 8000 AD.

1.2.4. Engineered barrier-related scenarios

Several scenarios consider different initial states, rates of degradation, and/or failure of particular engineered barriers, relative to the main scenario. These include accelerated degradation of concrete barriers, degradation of bentonite by formation of an ice lens in the silo during periglacial periods, and a future earthquake sufficiently strong to cause failure of the concrete barriers in the silo. The "high water flows in repository" scenario assumes that all concrete and bentonite in the waste vaults and plugs have a hydraulic conductivity of 10^{-3} m/s, which is very high relative to the expected properties. The case of an unclosed repository is also considered as an extreme case in which the repository is abandoned after most or all of the inventory is in place, without installing the engineered barriers that would be installed as part of the closure process.

The accelerated concrete degradation scenario (Main report, Section 9.3.3) produces up a 50% increase in annual dose relative to the main (global warming) scenario.

The calculated doses are not sufficient to exceed the risk criterion, but they approach within a factor of two. When this scenario is combined with high flow in bedrock is described (Main Report, Section 9.5.1). The peak annual dose approaches but is still below the dose corresponding to the risk criterion. The effects of the bentonite degradation scenario (Main Report, Section 9.3.4) are comparatively minor; the main influence is seen in terms of slightly increased doses beyond 20,000 AD.

A more extensive loss of barrier function in these barriers (as represented by the high water flow in repository scenario), the maximum dose increases by an order of magnitude, and exceeds the risk criterion. The scenario of an unclosed repository results in peak doses are 3 to 4 orders of magnitude above the risk criterion, depending on the assumed inventory at the time of abandonment. Together these scenarios show the importance of the engineered barriers for long-term safety of the repository.

The hydrogeological consequences of the earthquake scenario are based on an assumption that the concrete barriers in the silo fail, so water flow increases. The peak dose for this scenario is about three times as high as for the main (global warming) scenario, sufficient to exceed the dose corresponding to the risk criterion.

1.2.5. Future human actions

Scenarios involving future human actions are discussed in Section 7.7.7 of the Main Report. Actions discussed include:

- Drilling into the repository,
- Water management (removal or modifications to the SFR pier),
- Underground construction (tunnel or mine near repository),

Only the first of these is addressed quantitatively; the treatment focuses on exposure of a drilling crew or future activities on a drilling detritus landfill, which does not have a close relationship to hydrological issues. The other two categories of actions are said to be addressed qualitatively in the FHA Report (SKB TR-14-08), which has not been reviewed for this task. The qualitative discussion likely hinges on the hydrogeological modelling that was conducted for other purposes, including for the site descriptive model.

2. Assessment of SKB's presentation

2.1. Overall quality of documentation

2.1.1. Structure and transparency

The main SDM-PSU report, the bedrock hydrogeology report (SKB R-11-03) and the hydrogeological and surface hydrological modelling reports (SKB R-11-10 and SKB R-13-25) are generally well structured and are reasonably transparent. Assumptions and methods are generally well explained, particularly in explaining what combinations of variants were considered, and how these are defined. The tables of terminology and acronyms (for example Table 1-3 of SKB TR-11-03 and Table 1-4 of SKB TR-11-10) are especially helpful.

One weakness discussed further in the companion review (Geier, 2015) is that the main numerical model used for the deep hydrogeological system, DarcyTools, is explained only briefly as a series of equations solved, for example in Appendix A of SKB TR-13-25), and a very general summary in the Models summary report.

The description of bedrock hydrogeological modelling by Öhman et al. (2013) is detailed and thorough in terms of describing the different steps of modelling and the reasons for testing different variants. This report seems to have been less thoroughly edited for technical English than most of the other reports considered in this review, as it contains some unusual expressions (for example on p. 40 there is a discussion of the "hydraulic dignity" of SBA structures relative to the sheet joints encountered at Forsmark; presumably some other term such as "hydraulic rank" or "hydraulic order" was intended). However the technical assumptions, logical approach, and intended meanings are generally clear from the presentation.

2.1.2. Traceability

The SDM bedrock hydrogeology report (Öhman et al., 2012, Table 1-4) includes a list of data that were used, with reference to specific sources whether in SKB's Sicada database, tables in published reports, RVS or GIS models, or other specific SKB documents. The background reports describing analysis of interference tests (SKB P-10-43) and parameterization of the HCDs (SKB P-09-49) also give a clear account of the data used and the different steps and assumptions in the analysis.

Extensive appendices in both R-11-03 and R-11-10 document the details of analysis, submodels, model variants, and key datasets. These appendices appear to be sufficiently detailed to support more detailed reviews on most of the key topics. Links to analyses that are documented in the background (P-series) reports are also generally clear.

As one example, a more intensive review of SKB's use and interpretation of cross-hole responses to interference tests (in both "old" and "new" SFR datasets) could be well supported by information given in Appendices D and E of SKB R-11-03, Chapter 7 of SKB R-11-10, and the background report by Walger et al. (2010).

One area that is less traceable is the handling of uncertainties. The uncertainties identified by (Öhman et al., 2012) do not clearly map into the discussion of confidence and remaining uncertainties in Section 7.6 of the SDM-PSU main report. This is discussed further in Section 2.3.

2.1.3. Scientific soundness

The scientific approach employed in developing the bedrock hydrogeology portion of the site descriptive model is generally credible, in terms of the methods of analysis employed and the inferences drawn. However the descriptive model presented as the outcome is not mature to the level that should be expected for a safety assessment in support of a license application. Strengths and weaknesses of the scientific and technical development can be assessed in terms of the following major topics:

- Structural geological basis for hydrogeological models
- Analysis of hydraulic interference tests
- Analysis of trends and heterogeneity in hydraulic domains
- Treatment of bedrock fractures outside of deformation zones
- Understanding of processes limiting inflows to tunnels
- Consequences of inflow uncertainties for repository resaturation
- Hypothesis of hydraulic choking at sediment-fracture interface
- Overall maturity of site interpretation

These topics are discussed sequentially under the corresponding headings.

Structural geological basis for hydrogeological models

The structural geological interpretation as presented in Chapter 5 of SKB TR-11-04 guides the identification and classification of the large-scale and small scale structures that are the basis for the hydrogeological conceptual model in terms of HCDs and DFN models of the HRD, respectively. Much of the information is drawn from the structural geological model for SR-Site, but with more detailed attention to the areas that are currently offshore. Notable differences in terms of data support are the lack of outcrops at ground surface, but the availability of underground mapping data from the lower construction tunnel (NBT) in the SFR. As for SDM-Site, borehole logging with BIPS plays a major role in constraining the geometric properties of the DFN models.

Fractures that were mapped in the tunnel for SFR construction have been considered but their quantitative treatment is limited. According to TR-11-04 (p. 71-72), many of these are below the scale that is considered for deterministic modelling in the SDM, and some of the minor structures in the drawings of Christiansson and Bolvede (1987) do not meet current criteria as “possible deformation zones.” However the report states that all of the features in the structural drawings of Christiansson and Bolvede (1987) have been treated as “possible tunnel deformation zones (tPDZs). The treatment of these older data should be considered as part of a more detailed review of the completeness of SKB's use of relevant data to address uncertainties in the hydrogeological model.

Analysis of hydraulic interference tests

Walger et al. (2010) give evaluations of the pressure responses in all instrumented SFR-boreholes, in response to hydraulic perturbations due to four interference tests and due to the drilling of six boreholes (one of the four interference tests, in the shallow percussion-drilled borehole HFR102, produced no identifiable responses). The presentation is systematic and based on generally accepted principles of well-test analysis. Diagnostic plots and response matrices are included that are consistent with current scientific practices and give a sufficient basis for independent evaluation of the results.

The approaches to interpretation of these tests by Walger et al., (2010), as well as subsequent modelling of the propagation of pressure disturbance in a HCD network model by Öhman et al. (2013), appear to be technically sound and scientifically credible. However due to the significance for understanding hydraulic connections at the site, it is recommended that these data and interpretations be considered within a detailed-phase review of the hydrogeologic data and their application to parametrization of the hydraulic domains as discussed under the next heading.

Analysis of trends and heterogeneity in hydraulic domains

The analysis to support the concept of depth-dependent trends in the HCDs and HRD is described in detail by Öhman and Follin (2010, SKB P-10-43). This gives a detailed account of the interpretation of hydraulic data in terms of parameterizations for the HCDs and HRDs. The analysis is used to justify models for trends in hydraulic properties of these domains with depth.

The account is thorough and sufficient to support an external review of the details. The conclusions regarding trends are arguable but the analysis is transparent. Sensitivity to the classification of data as belonging to HCDs vs. HRDs is included.

The focus has been in terms of vertical trends, but a full consideration of possible lateral trends is lacking. Plots are presented of HCD variability in transmissivity with depth, but not along strike. For the HRD, a trend in depth is suggested but analysis of lateral trends is limited, particularly for the rock north of the SFR where data are very limited. Use of older data and data from partly-penetrating intervals appears to have been limited and non-systematic based on the discussion in Öhman et al. (2013).

The possibility of lateral trends in the HRDs is very briefly discussed and dismissed despite an apparent trend of increasing PFL-f transmissivities from the Central block toward the Northern boundary belt. The rationale given by Öhman et al., 2012 (pp. 109 and 114) is that confidence in the apparent trend is limited due to "borehole coverage gaps, sampling bias, and variable detection limits" in combination with the lack of packer test (PSS) data to assess the role of hydraulic chokes.

Öhman et al., 2012 (p. 107) mention both uncertain data quality and geometric uncertainties as a justification for excluding older data from evaluation of HCDs properties. The older data tended to indicate higher transmissivities for these HCDs. To the extent that this is a function of geometric uncertainties (presumably meaning that elevated transmissivities belonging to some intervals outside of a given HCD, for the current model, were assigned to that HCD in the earlier interpretation), this implies that the higher transmissivities should need to be taken up by the model for the HRD. This has not been done, as these older data were simply excluded.

A review is suggested of the uncertainties identified by Öhman et al. (2012, 2013), as well as independent interpretations of the underlying transmissivity data and trends. The datasets listing transmissivity values in all boreholes (both “old” and “new” datasets), and transient records of responses during interference tests, should be requested to support this type of analysis.

A more thorough review of the HCD and HRD parameterization is therefore suggested. This review should also consider whether all of the available data have been used as fully and effectively as is reasonably feasible to constrain the parametrization, or whether some of the older, lower-resolution data could provide further significant constraints on the model.

Treatment of bedrock fractures outside of deformation zones

Analysis of data to support an updated hydrogeological DFN model is presented mainly as an appendix (Appendix G) of Öhman et al. (2012). The methodology is similar to that employed for derivation of the corresponding models for SR-Site, but with less consideration of alternatives for fracture spatial models and the inferred relationship between fracture transmissivity T and fracture size (expressed as fracture effective radius r). Only a Poisson process for fracture location has been considered. Two different assumptions are tested for scaling of fracture size and intensity, but only one relationship between T and r has been evaluated, namely a perfect correlation of transmissivity to fracture size, $T = ar^b$. This contrasts with SR-Site where three different relationships between T and r were evaluated, and a fractal model for fracture location was tested.

Analysis of variation in fracture properties with depth has led to definition of three different depth zones in the DFN model. A corresponding analysis of spatial variation in the lateral direction is minimal (in part due to limited data support from north of the SFR), with just a brief consideration of differences between the two rock domains RFR01 and RFR02 (Öhman et al., 2012, p. 271-272). Details to support the conclusion of negligible difference between rock domains are not presented. The authors argue that it is difficult to ascertain differences due to “heterogeneity, data gaps, and sampling bias.”

The model for outside of the SFR regional domain comes from SDM-Site. There is practically no information from the northern boundary belt to support use of this model there.

Öhman et al. 2013 (p.37) present results for only one realization of the inferred DFN model for the HRD portion of the bedrock. Thus even within the framework of the derived DFN model, stochastic uncertainties have not been explored.

Sheet joints in the shallow bedrock have been treated both deterministically and with a stochastic model of the “shallow bedrock aquifer” (SBA) by Öhman et al. (2013, model case M7). The methods for developing the stochastic SBA model are acknowledged by Öhman et al. (2012) to be non-systematic in comparison with other stochastic fracture models developed by SKB in SDM-Site and SDM-PSU.

Thus it can only be regarded as illustrative rather than a quantitatively justified model. Only two realizations of this model are considered, so furthermore the illustrative application has been limited.
Further review of the DFN and SBA models, focusing on the potential significance for the safety case of unevaluated uncertainties, is therefore suggested.

Understanding of processes limiting inflows to tunnels

A key unresolved issue for site understanding is the reason for continuing decline in flow to the existing SFR vaults and tunnels, over time. Five possible mechanisms are suggested as explanations on p. 47 of SKB R-11-03:

- Heterogeneity and isolated/compartmentalized rock mass;
- Unsaturated fracture flow (possibly including degassing effects);
- Particle clogging due to transport of particles from seafloor sediments or existing fracture fillings;
- Fracture sealing due to chemical precipitation and microbial growth;
- Hydromechanical closure of fracture due to increasing effective normal stress as groundwater pressures drop in fractures close to the excavation.

However very little evidence is presented as to their quantitative impact, apart from a simple scoping calculation for hydro-mechanical closure due to drainage of a horizontal fracture.

Considering that the trend in inflow measurements has been generally downward with a fairly consistent trend over nearly three decades since SFR was constructed the late 1980s, it is worrisome that SKB does not have a more clear quantitative justification.

No data are presented to quantify the inferred "skin effect" that was used as a model calibration parameter by Holmén and Stigsson (2001), such as (for example) head measurements in probe holes drilled out from the walls of the underground tunnels. This seems to be a key unaddressed aspect of site understanding that SKB should have tried to investigate, at some point in the past 15 years if not sooner.

Consequences of inflow uncertainties for repository resaturation

An understanding of the reasons for the decline in flows, and the calibrated "skin effect," is important both for confidence in post-closure flows through the waste vaults, and evaluations of the duration and importance of the resaturation period after closure. The model calculations by Holmén and Stigsson (2001) are referred to in several of the supporting documents for SR-PSU (see companion review by Geier, 2015) as the basis for assuming that the resaturation period is sufficiently brief that an analysis of resaturation processes is unnecessary.

As noted by Öhman et al 2013 (p. 35), the Holmen and Stigsson (2001) model was based on a different structural model with fewer structures, and calibrated to 1997 inflow data which were 64% higher than the 2010 data used in SDM-PSU.

As complementary information, SKB should explain the impact of using this old model, as the basis for quantitative estimates of the resaturation period duration and as justification for omitting a more detailed analysis of the resaturation period.

Hypothesis of hydraulic choking at sediment-fracture interface

Öhman et al (2012, Section 4.7.1) propose a concept of “hydraulic choking” at fracture-sediment contacts, which is invoked to explain part of the apparent resistance to flow through seabed sediments into discrete fractures. The proposed “choking” effect is supposed to represent the resistance that results from convergence of flow from a porous continuum into sparse, discrete fractures that are highly transmissive but have small apertures. Scoping calculations of the effect are carried and used to justify a “skin factor” at the interface between HRD and HSD.

From a geological perspective, this conceptual model and its numerical implementation are based on an overly idealized view of discrete fractures, particularly highly transmissive fractures that reach the upper surface of the bedrock. Noting that the geological rate of erosion of the bedrock surface is very slow, such fractures have been exposed to many climate cycles in their current configuration, and hence tend to have a complex structure widening toward the bedrock surface, due to the effects of weathering, freeze-thaw cycles, and glacial plucking or scouring of rock fragments. Hence the convergence in the overlying sediments need not be so extreme, as there may be a funnelling effect in the complex, surficial portion of fractures.

Furthermore anisotropy of the sediments, with higher hydraulic conductivity in the horizontal direction, can be expected for shallow Baltic sediments in a relatively sheltered bay such as over the Forsmark site. The authors do acknowledge (on p. 80) that such a situation would reduce the “choking” effect, but the scoping calculations that they present are based on an isotropic model of the sediments.

This is likely not a major issue affecting the safety relevance. However its introduction as a justification for skin effects at the Quaternary-bedrock contact adds to the impression that the hydrogeological analysis for SDM-PSU is still at an exploratory stage, rather than representing a fully mature stage of descriptive modelling.

Overall maturity of site interpretation

The modelling study by Öhman et al. (2013) is well-explained as a step-by-step process of investigation, but the selection of model variants is ad hoc rather than systematic. The discussion of alternative interpretations seems more appropriate for an initial stage of SDM development rather than an exploration of the properties of the final bedrock hydrogeological interpretation for SDM-PSU. The conclusions of this study as presented in Chapter 8 of Öhman et al. (2013) discuss the different variants in terms of their ability to improve certain aspects of the model, but do not point to a clear “central” model parameterisation that is considered most likely to represent the important properties of the site for safety.

The main bedrock hydrogeology report (Öhman et al., 2012, SKB R-11-03) was published before the modelling report (Öhman et al., 2013), and references to the latter are limited. The conclusions of the main report are in the form of a qualitative discussion that mentions different alternatives, but does not go any further than the modelling report, in drawing together a clear statement of a “central” model.

In several places, the main bedrock hydrogeology report (Öhman et al., 2012) cites the lack of hydraulic packer-test (PSS) data to complement PFL-f measurements as a key factor limiting the understanding of the HRD. This apparent deficiency could have been remedied by a follow-up program of testing and analysis, but this was not done. The higher-level reports do not clarify whether this apparent deficiency identified in the analysis by SKB's consultants was dismissed based on scientific arguments, or simply ignored due to project schedule/budget constraints.

The weakness of the tunnel inflow data for discriminating among these variants is acknowledged by Öhman et al (2013). Heads in monitoring wells are also compared but without drawing clear conclusions. Systematic methods for optimizing the parameterization (such as response surface methods) in terms of its ability to reproduce the observations have not been employed.

Taken together, the reports on descriptive model development for bedrock hydrogeology reflect a very substantial amount of work to explore different possibilities, but which stopped short of producing an integrated model that weaves together the different threads of exploration.

The decision to proceed from this situation to modelling for a license application implies a need for SKB to provide a comprehensive assessment of unresolved hydrogeological model uncertainties, in support of SR-PSU.

2.2. Important data and assumptions

The most important data and assumptions that propagate from the hydrogeological analysis into the SR-PSU safety analysis are those that affect the estimation of groundwater flux through the vaults, and secondarily transport properties along discharge paths.

In the models presented by SKB within SDM-SFR, the key aspects affecting groundwater flux are:

- HCDs and their parameterisation;
- Effect of HSD layer, particularly seabed sediments and hypothesized "skin effects" at the HSD-HRD interface, for limiting fluxes at depth;
- SBA properties and their influence on limiting hydraulic head gradients at repository depth;
- HRD properties as represented by the stochastic DFN model; and
- Hypothesized tunnel skin effects and their persistence in the post-closure period.

Concerning the first of these, the HCDs have been a major focus of SKB's analysis. The details of this analysis are adequately presented to support detailed review.

The effects of the HSD layer and seabed HSD-HRD interface are likely most significant during the open repository period, and will become less important following closure and coastline retreat, when terrestrial processes are likely to reduce the resistance to vertical flow (either by erosion of the HSD or by bioturbation processes that increase vertical permeability), and regional flow driven by topography becomes more important. However assumptions regarding the HSD affect calibration of the bedrock hydrogeological model.

The SBA has been represented both by a set of 8 deterministic features and by a stochastic representation. Substantial uncertainty is associated with the role and extent of these features. However the model exercises presented by Öhman et al. (2013) provide a reasonably adequate basis for interpreting the potential impacts of these structures on repository fluxes.

The roles of the HRD properties and associated uncertainties are not fully clear from the analyses that have been presented, in part because of SKB's limited evaluation of conceptual and stochastic uncertainties associated with this domain. The residual flowrates into the SFR, following grouting of intersections between tunnels and the main HCDs, indicate that the role of the HRD is significant. However it could diminish after closure if HCDs become more dominant as grout degrades.

The skin effect attributed to open tunnels in the SFR could be regarded as an issue that mainly just affects model calibration, if the hypothesized explanations are correct and these effects are reversed following saturation. However even if this interpretation is correct, the persistence of the skin effect following closure could impact the duration of the resaturation period.

Conceptual uncertainty in the physical explanation for tunnel skin effects is high. This translates into substantial uncertainty in resaturation processes, which have mainly been discussed but not analysed by SKB.

2.3. Handling of uncertainties

The "hydrogeological" key issues identified by Öhman et al. (2012, Section 7.6) include most of the main uncertainties that are likely to be significant for groundwater flux and flow path properties affecting safety assessment calculations.

Uncertainty in HCDs and their parameterisation has been the subject of considerable attention in SKB's hydrogeological site-descriptive modelling. Several different alternative parameterizations involving depth dependency and heterogeneity have been evaluated in the modeling exercises, giving a reasonable basis for assessing the sensitivity insofar as these were propagated to safety assessment.

Uncertainties in the HRD and SBA have been considered to a more limited extent, and therefore more detailed review of these aspects of SKB's site descriptive modelling is recommended. Öhman et al. (2012) recognize that residual uncertainties in terms of bedrock (HRD) connectivity may play a role in the apparent lack of steady-state conditions in response to excavation of the SFR.

The hydrogeological uncertainties identified by (Öhman et al., 2012) do not clearly map into the discussion of confidence and remaining uncertainties in Section 7.6 of the SDM-PSU main report (Table 1). Tracking and accounting for the handling of uncertainties from different stages of model development is recommended as a topic for further review. As input to such a review, it could be useful to request SKB's own accounting of how they have taken these uncertainties into account, as complementary information.

Table 1: Comparison of uncertainties/issues raised in bedrock hydrogeology report (SKB-11-03) versus handling in the SDM-PSU main report (SKB TR-11-04 Section 7.6).

Issue	As raised in SKB R-11-03	Handling in SDM-PSU main report
Hydraulic properties of HCDs	ENE to NNE and WNW to NW sets of deformation zones within the Central block are highly heterogeneous with local high-T channels; contact between ZFM871 and steeply dipping zones are highly heterogeneous; indications that ZFMNW0850B is heterogeneous and discontinuous.	No remarks on the significance of these inferences were found in this preliminary-stage review.
Hydraulic properties of HRD	Base-case parameterization is provided in Table 6-2; alternative parameterization including KFR106 is provided in Table G-7. Possible depletion of Hydro-DFN model by deterministic treatment of SBA structures is mentioned on p. 108 but not investigated.	No remarks on the significance of these inferences were found this preliminary-stage review.
Boundary of HRD domains for DFN model	Note on p. 109 that the boundary between the repository and deep domains may be need to be reconsidered once the depth of the SFR extension has been decided.	No remarks on the this topic were found this preliminary-stage review.
SBA structures	SBA8 is regarded as uncertain and not included in final model.	Eight SBA structures mentioned. No specific remarks on handling of uncertain structures such as SBA8.
Hypothesized absence of SBA structures below -60 m	Motivated by data from HFR101, KFR104 and KFR105, but not confirmed.	Not discussed.
Reliance on PFL-f data	Analysis relies exclusively on PFL-f data which are believed to be subject to “hydraulic choking” effects; packer test (PSS) data not available (p. 115) or not utilized due to questions about quality (p. 117).	Dependence of hydrogeological DFN model on PFL-f data noted (p. 180, 4th bullet) but discussion is limited to effects of transmissivity censoring.
Limited scope of interference tests	Intercepts of interpreted SBAs and unresolved PDZs have not been evaluated by interference tests.	Additional interference tests are discussed in relation to issue of declining inflows to existing SFR excavations.
Possible lateral trends in HRD.	Indications of possible trends especially in PFL-f transmissivity observed between the Central block and N/S boundary belts (p.	Possible lateral trends are mentioned as an uncertainty (p. 180).

	116). Various alternatives suggested in Section 5.6.	
Use of “old” data from the existing SFR	Older data seem to result in higher transmissivities of deformation zones, but only used as complementary data in SDM-SFR. Only core-drilled boreholes surveyed by PFL-f method used in SDM-SFR.	Historic and recent data noted to be of different quality and test types, and reflect different stages of the SFR disturbance; this complicates the use of a single model for different sub-domains. No discussion of plans for re-testing old boreholes.
Time-dependent decrease in inflow to existing SFR excavations	Alternative explanations raised but not quantified.	Acknowledged in general terms, but stated that of the possible reasons “probably all of them are reversible.” Suggested that further analysis of interference tests could shed light on this issue but due to short duration of these tests, calibration of storativity is a key issue. Longer-duration interference tests are mentioned as a way to provide more robust data but no plans to conduct such tests are indicated.
Uncertainties in SFR inflow measurements due to ventilation	Scoping calculations indicate significant impact of ventilation air.	Uncertainty acknowledged as +/- 30 liters per minute, depending on the season. No plans for measurements indicated.

3. Suggestions for further review

Several topics for further review have been identified in the foregoing chapters of this technical note. These are summarized here in terms of related topics that could be addressed most efficiently as integrated topics for the detailed review phase.

3.1. Parametrization of hydraulic domains

The parametrizations of the HCD and HRD are key for long-term flows to the waste vaults. Key uncertainties include the validity of interpreted trends with depth, the possibility of spatial trends in other dimensions or depending on lithological or structural domains which have been less thoroughly analysed, and the character of heterogeneity not explained by spatial trends.

A more thorough review of the HCD and HRD parametrisation is therefore recommended. This review should also consider whether all of the available data have been used as fully and effectively as is reasonably feasible to constrain the parametrization, or whether some of the older, lower-resolution data could provide further significant constraints on the model.

The datasets listing transmissivity values in all boreholes (both “old” and “new” datasets), and transient records of responses during interference tests, should be requested to support this type of analysis.

3.2. Stochastic models of transmissive fractures

The site-descriptive model development for bedrock geology includes development of a quite elaborate DFN model for the hydraulic rock domain (HRD), as well as a more stylized stochastic model of highly transmissive, mainly subhorizontal fractures that are considered to be part of a shallow bedrock aquifer (SBA). The hydrogeological modelling within SDM-PSU and SR-PSU has considered only a very limited number of realizations of these models, leaving questions as to the significance of their stochastic properties. In addition, uncertainties are associated with assumptions that were introduced in deriving these models, particularly for the stochastic SBA model.

Further review of the DFN and SBA models, focusing on the potential significance for the safety case of unevaluated uncertainties including stochastic variation, is therefore suggested. The utilization of relevant hydro-structural information from the SFR construction should also be examined, as part of this assessment.

3.3. “Hydraulic chokes” in the rock mass

The concept of “hydraulic chokes” in the fracture network in the rock mass in between HCDs is raised repeatedly in the documents considered for this review. The lack of usable data from packer tests, to complement PFL-f measurements, is mentioned repeatedly as a shortcoming of the site-characterization dataset that precludes resolution of this issue.

An independent evaluation of this issue is warranted. This should address firstly whether the interpreted hydro-DFN model of the rock mass leads to “hydraulic chokes" sufficient to explain SKB's explanations, and secondly whether a channelized network model would lead to a significantly different interpretation of the results.

3.4. Processes influencing inflows and resaturation

The conceptual as well as quantitative understanding of processes affecting time-dependent inflows to tunnels in the existing SFR is very weak. SKB should be requested to give a more thorough accounting of these processes and the related uncertainties, with an evaluation of consequent uncertainties regarding resaturation of the proposed facilities, and subsequent flows through the vaults. An independent review of the same topic is warranted to prepare for SKB's response.

4. References

Bosson, E., Gustafsson, L-G., and Sassner, M., 2008. Numerical modelling of surface hydrology and near-surface hydrogeology at Forsmark. Site descriptive modelling, SDM-Site Forsmark, SKB R-08-09, Swedish Nuclear Fuel & Waste Management Co.

Bosson, E., Sassner, M., Sabel, U., and Gustafsson, L-G., 2008. Modelling present and future hydrology and solute transport at Forsmark. SR-Site Biosphere, SKB R-10-02, Swedish Nuclear Fuel & Waste Management Co.

Christiansson, R., and Bolvede, P., 1987. Byggnadsgeologisk uppföljning, Slutrapport. SKB SFR 87-03, Swedish Nuclear Fuel & Waste Management Co.

Dershowitz, W.S., Lee, G., Geier, J., Foxford, T., La Pointe, P., and Thomas, A., 1998. FracMan interactive discrete-feature data analysis, geometric modeling and exploration simulation. User documentation version 2.6, Golder Associates Inc., Redmond, Washington.

Follin, S., 2008. Bedrock hydrogeology at Forsmark. Site descriptive modelling. SDM-Site Forsmark. SKB R-08-95, Swedish Nuclear Fuel & Waste Management Co.

Geier, J., 2015. Hydrogeological analysis in the safety assessment SR-PSU – Initial review phase. SSM draft report 15 Aug 2015.

Holmén, J.G., and Stigsson, M., 2001a. Modelling of future hydrogeological conditions at SFR. SKB R-01-02, Swedish Nuclear Fuel & Waste Management Co.

Holmén J. and, Stigsson, M., 2001b. Details of predicted flow in deposition tunnels at SFR, Forsmark. SKB R-01-21, Swedish Nuclear Fuel & Waste Management Co.

Holmén, J.G., Stigsson, M., Marsic, N., and Gylling, B., 2003. Modelling of groundwater flow and flow paths for a large regional domain in northeast Uppland: A three-dimensional, mathematical modelling of groundwater flows and flow paths on a super-regional scale for different complexity levels of the flow domain, SKB R-03-24, Swedish Nuclear Fuel & Waste Management Co.

Johansson, P-O. 2008. Description of surface hydrology and near-surface hydrogeology at Forsmark. Site descriptive modelling, SDM-Site Forsmark, SKB R-08-08, Swedish Nuclear Fuel & Waste Management Co.

Mårtensson, E., and Gustafsson, L-G., 2010. Hydrological and hydrogeological effects of an open repository in Forsmark: Final MIKE SHE flow modelling results for the Environmental Impact Assessment, SKB R-10-18, Swedish Nuclear Fuel & Waste Management Co.

Mårtensson, E., Gustafsson, L-G., Aneljung, M., and Sabel, U., 2010. Hydrologiska och hydrogeologiska effekter på våtmarker och skogsområden av slutförvarsanläggningen i Forsmark: Resultat från modellering med MIKE SHE. SKB R-10-19, Swedish Nuclear Fuel & Waste Management Co.

Olofsson, I., Simeonov, A., Stigsson, M., Stephens, M., Follin, S., Nilsson, A-C., Röshoff, K., Lindberg, U., Lanaro, F., and Fredriksson, L., 2007. Site descriptive modelling Forsmark, stage 2.2. A fracture domain concept as a basis for the statistical modelling of fractures and minor deformation zones, and interdisciplinary coordination. SKB R-07-15, Swedish Nuclear Fuel & Waste Management Co.

Rhén, I., Follin, S., and Hermanson, J., 2003. Hydrological Site Descriptive Model – a strategy for its development during Site Investigations. SKB R-03-08, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., 2010. DarcyTools version 3.4, Verification, validation and demonstration. SKB R-10-71, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., and Ferry, M., 2010. DarcyTools version 3.4, User's Guide. SKB R-10-72, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., Ferry, M., and Kuylenstierna, H-O, 2010. DarcyTools version 3.4. Concepts, methods and equations. SKB R-07-38, Swedish Nuclear Fuel & Waste Management Co.

Werner et al., 2013. Hydrology and near-surface hydrogeology at Forsmark – synthesis for the SR-PSU project. SKB R-13-19.

Öhman, J., Follin, S., and Odén, M., 2014. SR-PSU Hydrogeological modelling. TD11 – Temperate climate conditions. SKB P-14-04.

Öhman, J., and Vidstrand, P., 2014. SR-PSU Bedrock hydrogeology. 0TD12 - Water-supply wells in rock. SKB P-14-05.

Reports included in review assignment

Abarca et al., 2013. Flow modelling on the repository scale for the safety assessment SR-PSU. SKB TR-13-08

Odén et al., 2014. SR-PSU Bedrock hydrogeology. Groundwater flow modelling methodology, setup and results. SKB R-13-25.

SKB, 2011. Site description of the SFR area at Forsmark at completion of the site investigation phase. SDM-PSU Forsmark. SKB TR-11-04.

SKB, 2013a. Climate and climate-related issues for the safety assessment SR-PSU. SKB TR-13-05 (published in October 2014).

SKB, 2013b. Bedrock hydrogeology - Groundwater flow modelling. Site investigation SFR. SKB R-11-10.

SKB, 2014a. Safety analysis for SFR long-term safety main report for the safety assessment SR-PSU. SKB TR-14-01.

SKB, 2014b. Initial state report for the safety assessment SR-PSU. SKB TR-14-02.

SKB, 2014c. Waste form and packaging process report for the safety assessment SR-PSU. SKB TR-14-03.

SKB, 2014d. Engineered barrier process report for the safety assessment SR-PSU. SKB TR-14-04.

SKB, 2014e. Geosphere process report for the safety assessment SR-PSU. SKB TR-14-05.

SKB, 2014e. FEP report for the safety assessment SR-PSU. SKB TR-14-07.

SKB, 2014f. Radionuclide transport and dose calculations for the safety assessment SR-PSU. SKB TR-14-09.

SKB, 2014g. Model summary report for the safety assessment SR-PSU. SKB TR-14-11.

SKB, 2014h. Input data report for the safety assessment SR-PSU, SKB TR-14-12.

Vidstrand, P., Follin, S., and Öhman, J., 2014. SR-PSU Hydrogeological modelling. TD13 - Periglacial climate conditions. SKB P-14-06.

Walger, E., Ludvigson, J-E., and Gentzschein, B., 2010. SFR Site Investigation. Evaluation of selected interference tests and pressure responses during drilling at SFR. SKB P-10-43.

Öhman, J., Bockgård, N., and Follin, S., 2012. Bedrock hydrogeology. Site investigation SFR. SKB R-11-03.

Öhman, J., Follin, S., and Odén, M., 2013. Bedrock hydrogeology. Groundwater flow modelling. Site investigation SFR. SKB R-11-10.

APPENDIX 1

Coverage of SKB reports

The following reports have been covered in the review (Table A1:1).

Table A1:1 Reports covered in review.

Reviewed report	Reviewed sections	Comments
SKB TR-11-04 Site description of the SFR area at Forsmark at completion of the site investigation phase. SDM-PSU Forsmark	All	
SKB R-11-03 Bedrock hydrogeology. Site investigation SFR	All	
SKB R-11-10 Bedrock hydrogeology - Groundwater flow modelling. Site investigation SFR	All	
SKB P-14-04 SR-PSU Hydrogeological modelling. TD11 – Temperate climate conditions.	All	Brief review; gives details of models presented in R-13-25.
SKB P-14-05 SR-PSU Bedrock hydrogeology. 0TD12 - Water-supply wells in rock	All	Brief review; gives details of models for well scenarios.
SKB P-14-06 SR-PSU Hydrogeological modelling. TD13 - Periglacial climate conditions	All	Brief review; gives details of models presented in R-13-25.
SKB P-10-43 SFR Site investigation. Evaluation of selected interference tests and pressure responses during drilling at SFR	All	
SKB R-13-19 Hydrology and near-surface hydrogeology at Forsmark – synthesis for the SR-PSU project.	All	
SKB R-08-67 Geovetenskapligt undersökningsprogram för	Chapter 7 (hydrogeology)	Chapters 3, 4 and 5 on investigation strategy, drilling program and geology also

utbyggnad av SFR (in Swedish).		skimmed for background.
SKB P-09-49 Site investigation SFR. Hydrogeological modelling of SFR. Data review and parameterisation of model version 0.1	All	
SKB TR-13-08 Flow modelling on the repository scale for the safety assessment SR-PSU.	All	Focus of separate review of SR-PSU; here as background to provide safety-assessment context.
SKB TR-14-01 Safety analysis for SFR long-term safety main report for the safety assessment SR-PSU.	All	Focus of separate review of SR-PSU; here as background to provide safety-assessment context.
SKB TR-14-02 Initial state report for the safety assessment SR-PSU	Sections on hydrogeological variables under 12.1.x – 12.8.x	Focus of separate review of SR-PSU; here as background.
SKB TR-14-05 Geosphere process report for the safety assessment SR-PSU	Section 3 hydraulic processes	Focus of separate review of SR-PSU; here as background.
SKB R-13-25 SR-PSU Bedrock hydrogeology. Groundwater flow modelling methodology, setup and results	All	Focus of separate review of SR-PSU; here as background to provide safety-assessment context.
SKB TR-14-09 Radionuclide transport and dose calculations for the safety assessment SR-PSU	All	Used here only as background regarding use of hydrogeological results in transport models for SR-PSU.
SKB TR-14-12 Input data report for the safety assessment SR-PSU	Hydrology-related AMF items.	Used here only as background regarding use of hydrogeological results in SR-PSU.
SKB TR-14-07 FEP report for the safety assessment SR-PSU	Hydrology-related FEPs only.	Used as background for review.
SKB TR-14-11 Model summary report for the safety assessment SR-PSU	Sections on DarcyTools, COMSOL, Ecolego and MIKE-SHE models.	Used as background for review.

APPENDIX 2

Suggested needs for complementary information from SKB

Requests for the following complementary information are suggested. The first three items could likely be satisfied by a brief memorandum from SKB giving links to the datasets on SKB's server. The last three items will require a more detailed response.

1. Transmissivity and hydraulic conductivity values interpreted for all boreholes (both "new" and "old" boreholes) in order to permit independent assessment of spatial trends and lithological/structural associations.
2. Digital versions of the single-hole interpretations of lithology and possible deformation zones, to support analysis of the preceding data.
3. Time series for flow and drawdowns in pumping wells and observation wells, for the full set of pumping/interference tests conducted at the SFR site (both "new" and "old" datasets).
4. An explanation of why hydraulic packer tests have not been carried out to provide data to complement the PFL-f measurements, despite that the lack of such data is cited as a key uncertainty in assessing the role of "hydraulic chokes" in models of the HRD (Öhman et al., 2012). Is there a scientific basis or was this just for practical reasons of cost or schedule? Are there alternative lines of evidence that could help to constrain this issue as a key residual uncertainty in the hydrogeological conceptual model?
5. An explanation of the consequences of using the older model of Holmén and Stigsson (2001) model, which was based on an earlier structural model with fewer structures, and was calibrated to 1997 inflow data which were 64% higher than the 2010 data used in SDM-PSU, as the basis for estimating the duration of the resaturation period for the proposed facility, and as justification for omitting a more detailed analysis of the resaturation period.
6. An inventory of uncertainties in the bedrock hydrogeological model identified by Öhman et al. (2012), showing whether and how these have been accounted for in the hydrogeological modelling for SR-PSU, and with an accounting of the expected consequences in terms of uncertainties in safety assessment calculations, for the uncertainties that have not been explicitly addressed.

APPENDIX 3

Suggested review topics for SSM

The following topics are suggested for review.

1. Assessment of SKB's parametrization of the HCD and HRD domains, focusing on the inferred spatial trends as well as the sufficiency of consideration of possible relationships to lithology and structures. This review should also consider whether all of the available data have been used as fully and effectively as is reasonably feasible to constrain the parametrization.
2. Assessment of the hydrogeological DFN and SBA models, focusing on the potential significance for the safety case of unevaluated uncertainties including stochastic variation. Utilization of hydro-structural information from the SFR construction should be examined as part of this assessment.
3. Review of the conceptual as well as quantitative understanding of processes affecting inflows to tunnels in the existing SFR, and consequent uncertainties regarding resaturation of the proposed facilities, and subsequent flows through the vaults.
4. A review of SKB's tracking and addressing of uncertainties that were identified in the analyses of bedrock hydrogeology for the site-descriptive model.

2

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Review of hydrogeological site-descriptive model SDM-PSU – 2

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Registration number: SSM2015-1017
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Abstract

This report presents a review of the hydrogeology and associated hydrogeological modelling undertaken in support of the licence application for the extension of the existing Swedish repository for short lived, low and intermediate level radioactive waste (SFR).

The overall conclusion is that the reports present a comprehensive Site Descriptive Model (SDM) that is well supported by data. The data collected represents a comprehensive compilation of the data that could be obtained from site investigation and development of the facility, and, whilst it can always be argued that additional data collection could improve understanding, it is considered that the data presented is sufficient to develop and give confidence in the SDM for the purposes of the licence application. The data comes from a long period of investigation for the SFR and Forsmark. Reporting shows data have been carefully and consistently integrated, as appropriate for developing confidence in the SDM.

The groundwater modelling delivers a prediction of the performance measures required for a safety assessment of the proposed extension of SFR, and these measures are considered appropriate to the level of detail used in the safety assessment modelling. The presentation is comprehensive in most areas and transparent; giving the reviewers a high level of confidence in the conclusions drawn by SKB and in the subsequent use of model results elsewhere in the licence application.

Some aspects of the modelling are acknowledged to not fully explain all aspects of the site, and in particular, the transient behaviour of the tunnel inflows is not fully explained. This is acknowledged by SKB and they present arguments why they consider that their understanding nevertheless is able to support the conclusions and results that they rely upon in their licence application. This review document suggests that additional parameter constraining value can be extracted from transient calibration of the bedrock model.

The main limitation in the SDM and the groundwater modelling is in the presentation of the treatment of heterogeneity and parameter and conceptual uncertainty. It is recognised that we have reviewed only a subset of the complete documentation and this aspect may be addressed in more detail elsewhere. Nevertheless, the reviewers would have welcomed a more explicit presentation of the SDM uncertainty as part of the SDM. It would also allow a more formal calibration process to be followed and in particular, target measures of the performance of the hydrogeological system could be identified and success criteria established so that it is clear when modelling and site investigation fully addresses the requirements of SKB's licence application to SSM.

It would also have been helpful to have presented more detail on water balances for the model. This would give a general hydrogeological description of the bulk behaviour of the Site Descriptive Model in terms that would be familiar to the wider hydrogeological community outside the nuclear industry. It would confirm the overall model is hydrogeologically consistent with a basic understanding of such hydrogeological settings.

Detailed issues worth further investigation are identified in the appendices.

Contents

1. Overview

This report presents a review of the hydrogeology and associated hydrogeological modelling undertaken in support of the licence application for the extension of the existing Swedish repository for short lived, low and intermediate level radioactive waste (SFR). Extension. The reports reviewed are detailed in Appendix 1 and subsequent sections of this report present the review of the key reports in turn.

The hydrogeological model presents the future site hydrogeology as a saturated, fractured granite bedrock that is intersected by a deformation zone of more intense fracturing and higher permeability, overlain by a thin, low relief regolith. The current SFR site is largely beneath a shallow part of the Baltic Sea, which is continuing to retreat as the region undergoes uplift in response to deglaciation. Future stresses to the hydrogeological system have been assessed via an ensemble of climatic and Baltic shoreline retreat scenarios.

The groundwater modelling delivers a prediction of the performance measures required for a safety assessment of the proposed extension of SFR, and these measures are considered appropriate to the level of detail used in the safety assessment modelling.

The reports are well written and provide a comprehensive presentation of the site.

An overall conceptual model was developed for the initial phase of the SFR and the Forsmark spent fuel repository. Recent additional investigations have been carried out to validate this model and to support an application to extend the SFR repository. Nevertheless, as is acknowledged in the reports, some aspects of the original conceptual model remain uncertain and the numerical modelling has been unable to reproduce all features of the site characterisation convincingly. This is as expected, since a conceptual model of the hydrogeology of the site is an ongoing presentation of the current state of understanding; this model should continue to be up-dated and tested throughout the project. SRK note that there has been a very open and honest appraisal of the shortcomings of some aspects of the modelling in several reports, which is welcomed.

The conceptual model (or Site Descriptive Model) has a number of audiences.
It needs to:

- present key performance measures needed by the Safety Assessment;
- inform ongoing operation and development of the site;
- guide future site characterisation work for the operator; and,
- demonstrate an understanding of the site to regulators, to a wider audience of nuclear industry specialists and further technical and lay communities.

It addresses the first three of these objectives well. However, as presented in the reports reviewed, the Conceptual Model is rather different to what many hydrogeologists, particularly outside the nuclear industry, would look for. A key issue is the limited extent to which the conceptual model is challenged. Data is interpreted in the context of the existing conceptual model, and where data does not fit, it is assumed to relate to as yet unmeasured detail within the existing conceptual framework or to permit additional elaboration of the conceptual model.

Water balances are rarely presented and a recurring recommendation in this review is to present conceptual and simulated water balances. This inclusion would provide reassurance that simulations are capable of representing regional scale conceptual flows, help to constrain large-scale saturated formation properties and permit cross comparison of various modelling approaches e.g. recharge in near surface models and boundary condition fluxes used in bedrock modelling.

The presentation of uncertainty is sparse; particularly parameter uncertainty. It would be helpful for the conceptual model to present ranges of uncertainty for input parameters and for parameters that the model's key output metrics are most sensitive to, be identified within the modelling reports, and that this sensitivity also be quantified.

In addition, there is limited discussion on conceptual uncertainty and alternative concepts. Where data are divided between features or zones, there is no presentation of rigorous statistical tests to confirm the distinct datasets. There are outstanding questions as to whether new data support the increase in the number of distinct parameter zones within the models with the presented material. New data appears to have been used to parameterise properties of the existing conceptual model rather than to test these assumptions.

It is implied that there is a wealth of transient data which could be utilised in future refinement of models. It is surprising that many of the simulations are steady state given that the SFR repository has been in operation for decades and that there now exists a considerable body of spatial and time-variant, regional head data with which to calibrate the transient condition.
Whilst it is recognised that the safety case will likely be determined by long term steady-state flows, it is suggested that transient simulation of these data at regional scale could provide valuable constraints on repository-scale bulk permeability and storage. This would add significant confidence to rock parameterisation and therefore through-flow estimates under future climatic or shoreline regimes.

The extent to which there is uncertainty in data or engineering from earlier phases of the project is surprising. There has been work to consider how best to maintain knowledge of the repository over the thousands of years when the repository continues to pose a potential hazard. However, the integration of datasets from only 20 years of continuous investigation and development has revealed a significant loss of knowledge from early stages (for example relating to tunnel wall exposures and drainage engineering).

Finally, a minor comment on reporting is that whilst the consistent internal nomenclature helps maintain data quality across multiple phases of investigation, the long and similar references for HCD structures, for example, makes these reports difficult to read. The diagrams presenting three-dimensional distribution of properties or responses are also difficult to read; fence diagrams or projected sections are easier to interpret. Quite a number of scanned figures are of poor quality when printed.

2. Site Descriptive Model [SKB TR-11-04]

The Site Descriptive Model (SDM) constitutes a comprehensive and consistent presentation of what is known about the site.

The SDM is interpreted as an extension of previous characterisation undertaken for the SFR and for the spent fuel repository programme. These prior studies are clearly well integrated into the current work. At this level of review it is considered that care has been taken to ensure consistency of approach when incorporating older datasets.

It is recognised that lack of access to tunnel rock, surface exposures and general sub-sea location results in characterisation challenges. Specifically, characterisation challenges exist for bedrock as data typically derives from discrete, single borehole observations. This limits what can be determined about the scale and connectedness of features.

A number of alternative numerical models are presented in the SR-PSU Hydrogeological Modelling report (SKB P-14-04) and the Bedrock Hydrogeology – Groundwater flow modelling report (SKB R-10-11) but these simulations are focussed on the Regional scale model which is quite small relative to the overall flow system. They are based on the existing conceptual model and so address uncertainty associated with heterogeneity of features within the existing interpretation.

A more rigorous treatment and presentation of uncertainty would be worthwhile, addressing parameter uncertainty more generally. That is, considering the range of values parameters used to specify the stochastic models might take, as well as considering the range of outcomes due to stochastic simulation of heterogeneous structures and selection of specific realisations; other sections of the review address this issue.

The conceptual model for SFR is also considered to be an extension of prior site characterisation, and new data is appropriately incorporated by refining parameters, or by increasing the number, and detail, of distinct sub-domains. However, the trend of producing increasingly detailed sub-domains is not assessed statistically in the reporting. Many of the trends appear weak compared to the dataset variability and therefore it is recommended that a more formal statistical approach is adopted to test the significance of such sub-classifications and trends to justify this approach. At this level of review, it should be noted that there is no suggestion of inappropriate use of data; recent sub-domains could be a positive evolution of past works. However, the field data may not be sufficiently robust to constrain the newly enhanced sub-domain discretisation. Statistical testing would help to define and justify the degree of parameterisation possible with existing datasets.

There is limited discussion of alternative conceptual models. For example, PDZs could simply be variability in bedrock properties or flow within deformation zones where there is strong channelling and one-dimensional flow. Of potentially greater significance was the absence of any discussion on quantitative uncertainty in the SDU. In particular, there is no mention of confidence tests for the classification of features and domains, or tabulated ranges of uncertainty associated with model input parameters. These can often be bounded using other data, for example, observed head gradients can constrain transmissivity across the site when considered in conjunction with the overall water balance. Equally, the presence of recent water e.g. 3H evidence will confirm the presence of rapid transport pathways and of fluxes through the system.

The site exhibits some significant differences from the Forsmark site to the south, particularly in the description of the shallow bedrock. Given this, it would be instructive to give more consideration to conditions further inland, particularly as this area defines the boundary conditions for groundwater flow through the site. Is the SFR site typical? Or are conditions at Forsmark typical? Are there larger scale structures compartmentalising the groundwater system?

3. Hydrogeological Modelling [SKB P-14-04] & Hydrology and near surface hydrogeology [SKB R-13-19]

Comments specific to the bedrock hydrogeological modelling are located in Section 4.

It is suggested that mass balance, solver convergence and grid convergence checks are incorporated into modelling reports. This comment is common to all reviewed modelling documents. Without these data it is only assumed during this review that models do not have instabilities or mass discrepancies. This is an uncomfortable position. This suggestion is important for all models that are used in this study, but particularly where such models exhibit large property variations. It would be reassuring to see that simulated results of concern were not influenced by the discretisation, solver convergence characteristics or general model mass discrepancies. Furthermore, the reporting of mass balance would provide indirect reassurance of modelling code capabilities.

In presenting the future modelling over long timescales it is anticipated that genuine transient models would be applied as opposed to a sequence of steady-state snapshots. Whilst issues of ongoing rebound are clearly complex, they could be represented quite simply by time varying boundary conditions. In particular, the F-quotient is typically many thousands of years per meter, yet these are presented in a sequence of steady state flow fields spaced with intervals of the order of 2000 years, during which the boundary conditions and path lines change significantly. If additional modelling is undertaken to investigate this point, it is not proposed that long-term transient simulation should be implemented in an onerous manner. The potential changing climatic and sea level regimes can be done using a simple transition in boundary condition parameterisation, as would be appropriate for the large uncertainties in future climatic and shoreline details.

The modelling reported in this document applies recharge directly to the model, whereas the Bedrock Hydrogeology Modelling uses constant head boundaries. It is not clear how consistent the models water influx volumes are in each of the reported setups. Reporting demonstrating similar water balances would provide additional credibility to the ensemble of models applied.

The model domains extend over surface water catchments, but these do not always correspond to groundwater catchments. Of note however, the SFR local and regional domains are relatively small in extent. The model properties outside the SFR Regional domain are simplified and assigned constant properties. The edge boundaries here are anticipated to impose controls over the metrics which the model is designed to predict. From initial review it is considered that the sensitivity of model predictions to edge boundary changes has not been investigated to the same extent as details within the SFR regional model. Whilst more distant properties will have a less direct influence on the performance measures predicted, these properties and the boundary conditions determine the groundwater fluxes into the SFR Regional Domain and are considered to strongly constrain results within the more detailed domain, regardless of how wide ranging the sensitivity analysis is within the SFR Regional Domain. Thus, a range of alternative simulations have been selected for sensitivity analysis in section 4 of SKB P-14-04, these address alternative descriptions within the SFR regional domain, in order to predict the range of fluxes and pathlines through the SFR tunnels and vaults However, section 4.3 of the report presents the common parameterisation of the model outside the SFR Regional Domain out to the flow boundaries of the Flow Domain. This common description of the outer part of the model, connecting to the flow boundaries, will limit the range of model outcomes, particularly for post closure simulations. This in turn would lead to the sensitivity analysis failing to identify the full range of outcomes associated with the SDM when accounting for parameter uncertainty over the Flow Domain.

It is further suggested that consideration of groundwater catchment boundaries on a larger scale might be worthwhile, particularly for later times when the Baltic is suggested to have retreated significantly from the site. Under this regime the hydrogeology could be controlled by more distant groundwater catchments.

In general, when selecting modelling tools, there is a tension between wanting to use the most appropriate and realistic representation (typically requiring specialist and custom developed software), and the reassurance of accuracy that comes with using a standard software tool that has been extensively and successfully used elsewhere. Darcytools is relatively new and the authors of this review are not aware of its use outside the nuclear industry. In addition, it was honestly and usefully reported that a bug in the DarcyTools code was identified during the modelling assignment. Given that, for example, Connectflow has been applied to this setting, it would be reassuring to see Darcytools model the same system as Connectflow (or vice versa) to verify that both codes produce similar results when applied to the same SDM. Whilst Darcytools has undergone verification and validation, it would be reassuring to see some direct code comparison in the SFR model scale and context.

If model code comparisons were undertaken, a review of differences in flow fields between pure Discrete Fracture Networks (DFN) and upscaling DFN to Equivalent Porous Media (EPM) models would add value. It is noted that extracting the connectivity and heterogeneity of the DFN through up-scaling to EPM affords a much more efficient computation and is considered a sensible approach.

Within the modelling approach applied here, the role of DFN modelling is to provide a description of the heterogeneity of flow paths through the Bedrock Hydraulic Rock Domain (HRD) which can then be upscaled to an ECPM. This has been implemented in the modelling by upscaling from selected stochastic DFN simulations undertaken in Fracman. The approach of using a relatively small number of selected realisations in the heterogeneous ECPM is reasonable, and section 4.2 identifies three Fracman realisations (R03, R18, and R85) to be used for upscaling to ECPM models in Darcytools. These were identified as either optimistic or pessimistic in terms of the intersections of fractures with SFR. However, it would be reassuring to demonstrate that the variation of performance measures (i.e. predicted fluxes and pathlines) in the Darcytools model that are to be used in safety assessment are consistent with the method used to select realisations of the DFN. For example, it is not clear that one can define statistics of the distribution of tunnel fluxes and particle travel times when the model is based on a very small number of stochastic realisations of the flow properties. Similarly, the heterogeneous HCD scenarios are based on only two (R01 and R07) realisations of the HCD heterogeneity (discussed in section 4.3 of the report). When defining the distribution of fluxes and paths through the SFR for use in Performance Assessment, it is expected that a larger number of realisations might be required, or else the justification of the very small number of realisations considered should be presented in more detail.

This coupling between tools using DFN models to derive heterogeneity for ECPM could be demonstrated on smaller systems and DFN selection methodology more clearly justified.

The site hydrogeology is strongly influenced by discrete features at many scales, and does not behave as a simple equivalent porous medium. However, in describing the hydrogeology of the site to a wider audience, it can be useful to use porous medium analogies. As an example, it would be helpful to have a catchment water balance presented and show that this was explainable in terms of simple boundary conditions, realistic recharge and bulk hydraulic conductivity and storage parameters. Consistency with simple 'back of the envelope' calculations would provide reassurance that more detailed modelling is reasonable. The additional model detail and complexity then provides an understanding and explanation of the role of site detail. It allows natural analogue and independent types of data (groundwater chemistry for example) to be used to confirm the overall behaviour of the system.

4. Bedrock Hydrogeology [SKB R-11-03]

The bedrock hydrogeology is developed from many years of investigation at SFR and Forsmark. The earlier data have been carefully integrated with more recent data and differences in quality standards are clearly identified and appropriately treated. This has resulted in a very detailed description of the properties of the bedrock in the SFR region. As would be expected, a range of tools and methods have been used over the period of investigation and data from different characterisation methods are compared, with the most recent investigations focussed on the use of the PFL tool and PFL-f logging. The presentation of the hydrogeology focuses on discrete responses and flows in the context of the established conceptual model, and is largely in terms of steady state properties of the flow system. In this review it is considered that there would be value in further development of an understanding of the transient behaviour of the system over the period of investigation and that there should be greater emphasis in the presentation of the bulk behaviour of the system as a whole, to provide context for the discrete flows measured on the experimental programme.

No presentation of the water balance for the region, SFR regional domain or the SFR local domain has been found. It is recommended that this be one of the key descriptors of the site hydrogeology and subsequent tests of the numerical modelling.

Reporting implies that data has been interpreted in terms of the accepted Conceptual Model. Significant considerations of alternative concepts are not reported in the reviewed literature. For example, the allocation of borehole intervals with anomalously high fracture intensities has been accommodated as PDZs rather than reconsidering the nature of fracturing of the bedrock. Whilst this would seem a reasonable hypothesis, there does not appear to have been quantitative exploration of alternatives such as clustering of background fracturing. Indeed, much of the assessment of uncertainty has been by qualitative discussion and judgement as to the most likely explanation rather than by formally identifying variant conceptual scenarios or quantifying ranges of parameter uncertainty. Bedrock hydrogeological modelling therefore could be skewed towards a specific interpretation of the system.

There is limited opportunity for observation of fracture traces at depth, and the interpretation of the bedrock has focussed almost exclusively on borehole logging. This leaves considerable uncertainty in the fracture size distribution, and indeed the DZ and PDZ size distributions. This is a concern, as the size distributions are a critical parameter in determining the connectivity and effective bulk hydraulic properties. The reliance on a correlation between size and feature transmissivity is likely to be a highly probable assumption. Whist these correlation assumptions are not unreasonable, alternatives should be explored and tested against the overall performance of the system quantitatively. Has there been investigation into fracture properties onshore in the vicinity of the site? It may additionally be worth considering borehole testing onshore to assess how typical the SFR site properties are in relation to the Forsmark tectonic lens and onshore bedrock domains.

The challenges of fracture identification and classification, particularly at depth, are normal and data to constrain simulated flow properties will be subject to uncertainty. It is suggested that bulk, spatially aggregated, properties can be backed out of existing larger scale datasets (e.g. inflow data) to help reduce the uncertainties associated with fracture parameterisation.

It is perceived that there is a reliance on the PFL tool for flow logging and transmissivity measurement. This method focuses on longer range properties of connected fractures which have a good connection to the borehole. This has the potential to introduce bias, and exclude flowing fractures connected through ‘chokes’ in the DFN. A PFL focus could therefore lead to biased estimates of the hydraulic diffusivity and to missing the properties of the slower parts of the network. Some discussion could be added describing how a more channellised DFN would present itself to borehole observation and PFL logging. In particular how channelling would be expected in the larger fractures. It would be helpful to see more rigorous comparisons of what is inferred from PFL logging and from conventional packer testing. For example, figure 6.1 shows up to three orders of magnitude (factor of 1000) variation between PFL-f derived transmissivities in zone with the same packer test transmissivity.

There is a consistent tendency to ascribe relatively small differences in calculated aquifer characteristics to distinct categories of domain or populations of features. Whilst this may be the case, classifications are suggested to be demonstrated through more statistical testing. The use of these datasets is primarily in the numerical modelling of the groundwater flow, and so the key issue is whether the hydraulic properties of different domains or populations are shown to be significantly different statistically. At this level of review it is not clear whether the detailed domain discretisation can be justified with the existing field data.

The 20 year legacy of dewatering is a key opportunity for the bedrock hydrogeology understanding. In particular, it is possible to back-out hydrogeological properties from the inflow rate changes that are observed over time. The reduction of tunnel inflow over this period is to be expected and a range of explanations are offered. Geotechnical conceptual processes are primarily suggested. For example the unloading effects from excavation and head reductions imparting a reduction in fracture or pore space size. Although all suggested mechanisms are considered possible, and all, or most, likely to be in operation, we would ask why the inflow reductions are not primarily attributed to gradual head reductions and storage depletion. Given the low permeability of the background bedrock, it is also possible that the primary mechanism for reduced inflows is the slow evolution of hydraulic head gradients within the background bedrock. This theory can be tested using simple calculations based on larger scale bulk properties, taking into account the timescale which inflow to an underground opening would evolve. Combined evidence from the PFL-f logging suggests that a significant fraction of tunnel inflow is indeed from the averagely fractured rock, and estimates of hydraulic diffusivity suggest that timescales for the development of hydraulic gradients might be comparable to the timescales over which the tunnel inflow is changing.

As introduced above, the system is transient. There is an excellent long term drawdown test that is expected to demonstrate excellent geochemical signatures in addition to head evolution. It would be helpful to have increased discussion of site transient behaviour, specifically, presentation of hydrographs at key locations around the tunnels and the deformation zones, and backing out of properties from long term evolution. In discussion of two observed cross-hole tests, the hydraulic diffusivity is considered but there is a reluctance to use standard definitions related to continuum concepts. These standard definitions will certainly not offer exact, or necessarily even good matches to DFN observations, but they are a standard and familiar way for hydrogeologists to describe groundwater systems at larger scales. Just as with a pumping test, it is not how well the data matches a Theis curve that is most illuminating, but the way in which it deviates that tells us about non-uniform properties, the existence of flow boundaries, and the existence of well bore storage and skin. The use of a scaled, alternative to the standard definition of hydraulic diffusivity is unhelpful.

It is suggested that additional understanding of bedrock system flow characteristics can be gleaned from basic analysis of sea level fluctuation attenuation in hydrographs. This currently is not reported and could be a valuable supporting dataset.

The absence of large scale water balance estimation, transient effect representation and minimal hydrograph discussion are the dominant comments pertaining to the Bedrock Hydrogeology Report.

5. Bedrock Hydrogeological Modelling [SKB R-11-10]

The groundwater modelling needs to demonstrate that:

- it is correct (that is, the tools have been verified as correctly solving the equations);

- that the model(s) represent the specific site both in setup and calibration;
- that the model either does not display non-unique features (parameter combinations which are not constrained by field data) or, more probably, that non-unique features have been identified and commented on through alternative model realisations; and,
- uncertainty associated with the models predictions of key output metrics have been identified.

The groundwater modelling of the bedrock makes a good start towards accomplishing these objectives, but still reads like a work in progress in some respects.

5.1. Modelling tools verification and mass balance

As additionally commented in section 4, it is recognised that there has been verification of the Darcytools software; however, it is a suggestion that cross-comparisons of the base case (or something similar to the base case) is undertaken with an additional modelling tool. As Connectflow has already had some use at this site, this is anticipated to be the most appropriate choice. Supporting reasons for the comparison include:

a). Concerns with the spatial resolution of the flow solution, particularly at the boundary between refined and less well refined areas, as evidenced by the need to correct bugs during the study; and,

b). Darcytools is less widely used than other tools. It would be valuable to compare its output (directly on the scale and resolution of the models relied upon) with simulators used outside of Sweden. It is possible that such comparisons have been undertaken external to this study and literature for reference is already available, but such studies have not been identified by the reviewers.

There is no reporting pertaining to convergence checking. It is not always obvious that a solution is well grid-converged, especially for very heterogeneous systems such as this, and particularly for transient flow, particle tracking and contaminant transport applications. The reviewers have two concerns:

1. It is not clear whether the Darcytools interpretation of ECPM properties from the network has been converged with respect to the Darcytools cell size; nor
2. Whether the grid used by Darcytools has then been discretised sufficiently to resolve flows through the inferred heterogeneous system.

5.2. Site specific representation - model setup and calibration

As commented in conceptualisation water balance tabulation is expected and the model simulation equivalent would additionally be a useful check on hydrogeological modelling.

The calibration processes' match to field data is not always convincing and this is recognised by the authors who are perhaps a little too harsh in their appraisal of the model results. It is therefore suggested that further model calibration is undertaken and the documentation of a systematic approach would be an asset to the reporting.

Greater confidence in the model's representation of the site would be achieved by assessing parameter uncertainty, tabulating best estimate and credible ranges of key parameters, identifying observed data targets and their associated uncertainty, setting calibration goals, and following a formal, documented, systematic calibration approach. It is also considered that a wealth of transient data is available. Notwithstanding the uncertainty associated with tunnel inflow and complex processes related to the excavation disturbed zone, modelling these transients could be of substantial benefit to the constraint of bedrock modelling parameters.

The steady state calibration undertaken followed a trial and error approach which, whilst not unreasonable, does tend to tempt the modeller into ever more detailed corrections or extensions to the conceptual model, potentially leading ultimately to 'curve-fitting' the targets. Section 5 of the modelling report discusses the range of trial and error modifications to the model intended to improve the match. This could have been more convincingly presented in the context of a formal calibration process, testing alternative scenarios and optimising parameter values. Ultimately, without *a priori* objectives, the modelling concluded instead with a rather vague assertion that the model matched the data 'reasonably well'.

The transient performance of the background bedrock is not reported to have been investigated. The system is in a transient state with a clear strong transient response that could be modelled. In addition to the tunnel inflows, regional groundwater hydrographs should be available with which to calibrate the model. The transient inflow to the tunnel is considered to be the most critical dataset for future transient model representation. Most data available corresponds to heads and the tunnel inflow is a key control on the system. An excellent constraint of regional aquifer properties should be obtainable through approximate representation of the net tunnel flow and simulation of changes in regional groundwater levels during the development of the site. This said, the system is obviously non-unique due to the use of constant head boundary conditions and groundwater head calibration targets. The non-uniqueness would be significantly reduced by using a mix of groundwater flux and groundwater head boundaries and targets. Combined consideration of recharge flux (in a detailed water balance calculation) and tunnel fluxes, potentially alongside other data sources (e.g. H3) would reduce concern over non-uniqueness (as indeed is recognised in one of the model variants). In association with this, it would be reassuring to see any documentation of how reasonable the recharge fluxes to the model are in relation to the recharge calculations carried out for the HSD.

The use of a skin factor within the tunnel as a model variable is effectively a fitting parameter and seems to be used to compensate for calibration deficiencies as currently reported. In general, it is suggested that skin is not simulated, as the effect is highly localised and not considered to affect the key metrics the model is designed to inform. If however there are local areas where skin is supported directly by data and explanation, then it is a valid inclusion.

A discussion is formed around the transient tunnel inflow datasets pertaining to reasons for inflow reduction over time. Various geomechanical/poro-elastic, degassing and hydro-bio chemical processes are suggested. In this specific section there is a good discussion of alternative conceptual processes which could account for the reduction of inflows to the tunnel. All are considered potentially valid, but not exclusive and simpler hydrogeological explanations are thought to be more significant. The surprise is the discussion starts from a premise that within 25 years the system would have been expected to be in steady state. In addition to this the explanations for inflow reduction over time are (generally) focussed towards potential restriction of flows in the vicinity of the tunnels, not the larger scale hydrogeological regime. All discussed processes are considered valid and likely to play a role to an extent however from the data presented in figure 2-6 it is considered by this review that the basic calculation of inflow reduction over time presented by SKB is consistent with drawdown of regional hydraulic heads in a leaky (Baltic) system. Rather than SKB's assertion that the reduction in flow is associated with unknown complex processes, it is considered by this review that the primary mechanism for inflow reduction might be simply the gradual pressure dissipation and regional storage reduction, once the role of the HRD is fully accounted for. Simulation of this effect could provide a valuable bounding constraints on the regional properties which will assist the repository scale flux metrics the model is designed to predict.

The model is specified in terms of the conceptual model and it is implied that parameters arise from interpretation of data in the context of that conceptual model. There is no concern with this so long as alternative conceptual flow processes are considered where there is uncertainty. It would be reassuring to have alternative conceptual flow processes explored and reported on both conceptually and numerically. This is especially suggested where the data in support of the parameters are noted to be weak. In the DFN description, two correlations are potentially very significant: correlation of fracture size and transmissivity, and correlation of fracture transmissivity with depth. Both of these are reasonable, but the data to support the correlations are very limited. The data was used to infer power law coefficients to these but there was no significant sensitivity or uncertainty analysis or alternatives to these correlations presented. The assumptions presented in these two relationships are commonly applied in underground mining models as a best approximation when no better data exist. During underground excavation however, when better data becomes available, the variability of fissure flow typically does not conform well to this numerical design at local scales, at full site scale however weak relationships between depth and fracture frequency or permeabiity would be typical.

5.3. DFN Considerations

As discussed above, Fracman was used to define the DFN geometry for a small number of realisations which were upscaled to ECPM Darcytools models. Fracman was also used to simulate interference tests (section 6 of SKB R-11-10). For the transient interpretation of the interference tests and transient responses, the DFN was restricted to a representation of the main hydraulic conductors (ie the HCD). Restricting the Fracman calculations to transient modelling of the DZ and PDZ system is computationally much more efficient and would be expected to account for the main initial responses but will clearly not be able to account for the role of the background fracturing (HRD) which may be important. Nevertheless this presents a useful transient flow study. A concern is that again, there is a reliance on a specific correlation of hydraulic properties (similar to the points made in section 5.2 above) through the empirical equation relating T and S (equation 6.2 of SKB R-11-10) for the model. The justification is by reference to Rhen et al.'s work at Aspo (SKB TR-97-06). There is no presentation of any discrete fracture packer testing from SFR or Forsmark to support this empirical relationship. Furthermore, by considering such a small system, the results of stochastic simulations are inevitably very variable and it is difficult to draw conclusions other than that the system can behave in a wide range of ways.

The evidence from PFL-f data (see for example section 6.4.3 of SKB R-11-10) is that the background rock plays a significant role in the transient behaviour (77% of the PFL-f transmissivity coming from HRD which is neglected, as opposed to the HCD which is simulated), which was not represented, adding to the uncertainty in how to evaluate the results.

5.4. Additional Comments

The use of constant density in the model is probably reasonable so long as care is taken in choosing an appropriate density and interpreting head data in terms of that density system (i.e. not freshwater heads).

It is noted that one of the key outputs from the model is the distribution of pathlines through vaults. The pathline algorithm used is a simple approximate method that will be computationally very fast, but which will be rather approximate for coarse grids. Whilst the authors note that one of the effects of the algorithm is to introduce some dispersion which is expected in the physical system, it is not reassuring to have the dispersive process incorporated as an effect of the numerical grid resolution. A more exact calculation of pathlines would be expected, and the role of transverse and longitudinal dispersion to be incorporated into radionuclide transport calculations explicitly and with reference to estimates of the physical properties (supported by data if possible).

5.5. Summary

In general, presentation of a more holistic incorporation of uncertainties would add value to the existing work. The large scale conceptual uncertainties of Climate are considered to be well catered for in other reports, more local scale conceptual uncertainties however could be elaborated within bedrock hydrogeological modelling. An area of uncertainty which is considered to be under represented is parameter uncertainty, particularly the influence of uncertain correlated parameters and the sensitivity of model output metrics (disposal room cross flow, particle exit locations to the regolith, flow related transport resistance, and advective travel time along flow paths) to the model input parameters. To be truly useful however it is suggested that additional works in parameter uncertainties are constrained through transient head and flow calibration, and analysis of ancillary datasets including hydrochemistry and recharge / water balances. Stochastic realisation work undertaken to date is reviewed positively. It may however be that additional realisations are required for a more quantitative prediction of uncertainty in performance measures. Also, fracture geometry and transmissvity relationship assumptions are not tested and these may have a significant influence on model outputs.

6. Conclusions and recommendations

This report presents an initial review of the hydrogeology and hydrogeological modelling submitted by SKB to SSM in support of the licence application for the extension of SFR. The review is limited in scope in that it did not review the complete licence application. It has also been undertaken in order to identify issues deserving more in depth review and as such it has not, for example, fully appraised the arguments where these are in part based on further detailed or precursor studies reported elsewhere.

The overall conclusion is that the reports present a comprehensive Site Descriptive Model (SDM) that is well supported by data. The data collected represents a comprehensive compilation of the data that could be obtained from site investigation and development of the facility, and, whilst it can always be argued that additional data collection could improve understanding, it is considered that the data presented is sufficient to develop and give confidence in the SDM for the purposes of the licence application. The data comes from a long period of investigation for the SFR and Forsmark. The data has been very rigorously checked and datasets have been carefully and consistently integrated, as appropriate for developing confidence in the SDM.

The hydrogeological modelling represents a state-of-the-art approach and again is scientifically sound and at an appropriate stage to support the licence application.

The presentation is comprehensive and transparent, giving the reviewers a high level of confidence in the conclusions drawn by SKB and in the subsequent use of model results elsewhere in the licence application.

Some aspects of the modelling are acknowledged to not fully explain all aspects of the site, and in particular, the transient behaviour of the tunnel inflows is not fully explained. This is acknowledged by SKB and they present robust arguments why they consider that their understanding nevertheless is able to support the conclusions and results that they rely upon in their application.

The main limitation in the SDM and the groundwater modelling is in the presentation of the treatment of heterogeneity and parameter and conceptual uncertainty. It is recognised that we have reviewed only a subset of the complete documentation and this aspect may be addressed in more detail elsewhere. Nevertheless, the reviewers would have welcomed a more explicit presentation of the SDM uncertainty as part of the SDM. It would also allow a more formal calibration process to be followed and in particular, target measures of the performance of the hydrogeological system could be identified and success criteria established so that it is clear when modelling and site investigation fully addresses the requirements of SKB's licence application to SSM.

The presentation should address both conceptual uncertainty, which may be investigated using alternative model scenarios, and also parameter uncertainty. It would allow the existing conceptual model to be challenged and identify where future monitoring or experimental work might best be able to reduce uncertainty by differentiating between alternate conceptual representations of the site hydrogeology. Explicit presentation of ranges of parameter uncertainty would allow a more formal quantification of the corresponding uncertainty in the output metrics relied upon by the safety case.

The reviewers would also have welcomed some additional context to the presentation of the SDM in terms of water balances and the overall description of the site in conventional hydrogeological terminology. Whilst it is recognised that a discrete feature dominated system such as the bedrock at this site cannot be characterised simply in terms of a porous medium, it is nevertheless helpful to give an overview of the hydrogeological system in such terms, and to identify overall constraints on the system performance. This would, it is believed, help communicate the confidence SKB develop in their SDM to the wider hydrogeological community.

Finally, whilst it may be detailed elsewhere, there should be reference to basic model checks such as grid convergence, and model verification. The approach to upscaling taken in Darcytools is not universally accepted and indeed the issue of upscaling from DFN to ECPM is an ongoing research topic. It is considered that this could be more strongly justified by reference to verification or by cross comparison against alternative numerical models, especially as these have previously been applied to the Forsmark and SFR hydrogeological setting.

APPENDIX 1

Coverage of SKB reports

Following reports have been covered in the review.

Table 1

Reviewed report		Reviewed sections
SKB-TR-11-04	SR PSU Hydrogeological modelling – TD11 – Temperate climate conditions	Main body of text reviewed
SKB-P-14-04	Site description of the SFR area at Forsmark at completion of site investigation phase	Main body of text reviewed
SKB-R-11-03	Bedrock hydrogeology Site investigation SFR	Main body of text reviewed
SKB-R-11-10	Bedrock hydrogeology – groundwater flow modelling - Site investigation SFR	Main body of text reviewed
SKB-R-13-19	Hydrology and near-surface hydrogeology at Forsmark – synthesis for the SR-PSU project	Main body of text reviewed
SKB-R-10-03	Site investigation SFR Hydrogeological modelling of SFR Model version 0.2	Specific areas referenced
SKB-R-10-71	Darcy Tools version 3.4 User Guide.	Specific areas referenced
SKB-R-10-72	Darcy Tools version 3.4 User Guide.	Specific areas referenced

APPENDIX 2

Suggested needs for complementary information from SKB

1. Where are the acceptable ranges of uncertainty for model parameters presented. SKB R-11-10 Appendix A Table A.1 for example identified discrete adjusted T values for HCD intersections, and Table 3.2 gives HCD log T mean and standard deviation parameters, but there is no uncertainty associated with these log(Teff(0)) and σ(log(Teff(0))). Is the modelling a best estimate model?
2. Are the models fully converged without significant mass discrepancy? Similarly, the particle tracking should be shown to be converged with respect to time discretisation. Whilst it is clear that this has been considered in the discussion of the mesh size in for example section 4.2 of SKB R-11-10, there is no explicit check on these numerical convergence issues presented. This should be found in SKB R-11-10 or referenced there.
3. What are the acceptance criteria for the numerical models and where is it shown that the results are acceptable? For example SKB acknowledge that they have not demonstrated an understanding of the decline in tunnel inflow (SKB R-11-10 section 2.8). It is implicit that this is not unacceptable, but there is no explicit identification of what role the modelling of the tunnel inflow plays in support of the SDM. For example, SKB should identify what is required of the models that are presented in SKB R-11-10 section 5 and then be able to demonstrate that this has been achieved. The discussion in SKB R-11-10 section 8.1 suggests that some improvement in tunnel inflow prediction was required but the evaluation of the various model variants M0 to M7 is qualitative and there is no ab-initio target set for an acceptable match to tunnel inflow. How can it be concluded that the model inflow is acceptable, and that there is sufficient support for the revised parameterisation of the HCD to be incorporated in the SDM and used for predictions for the safety case.
4. SKB should be asked for water balances for the main models of SKB R-11-10 identifying balancing rainfall, runoff, recharge, discharge and cross boundary flows for HSD, HCD and HRD, at least at the scales of the Flow Domain, Regional Model and Local Model. This would confirm that obvious requirements that fluxes are reasonable and, for example, that given fixed head boundaries for the bedrock modelling, the recharge is appropriate with respect to precipitation. This should also be done for the different time slice models presented for the sea level retreat steady-state models of SKB P-14-04. A main reason for water balance requests is to compare the in- and outflows of the various models and assure similar, consistent values are applied.

APPENDIX 3

Suggested review topics for SSM

1. Treatment of uncertainty. As discussed in Appendix 2 there is limited presentation of formal uncertainty analysis. It would be worthwhile compiling a list of where uncertainty in key properties is considered and how this is taken forward. In many cases, parameters are estimated without uncertainty (for example the parameters of SKB R-11-10 table 3.4), and in other places options are considered and the best fit chosen based on judgement (e.g. the model cases of SKB R-11-10 section 5). It is assumed that uncertainty will be addressed separately in the risk calculations, and it would be worth reviewing how real uncertainty in parameter values is passed between the site data synthesis and the final risk calculations.
2. There is opportunity and need for transient modelling of the site. It is believed that simple scoping ECPM transient modelling, using bulk properties, would give further insight into the tunnel inflow and, separately, the evolution of the site over the timescales of the Baltic coastline retreat (which is comparable to some of the steady state model advective travel times). SKB might be asked to do this or it may be appropriate for SSM to construct some simple models to investigate the SDM performance and provide context and a 'reality check' on the more detailed SDM models. If these show that performance does depend on transient behaviour, or indicate for example that the tunnel inflow can be explained better by accounting for the role of the HRD, it might lead to further work by SKB to evaluate the sensitivity of model outputs to transient effects.
3. Approach to calibration and identification of modelling objectives. It would be useful to identify where SKB define the objectives for different components of their models, and how well they are able to meet them. Ideally, the objectives and acceptance criteria for a model would be defined at initiation and then it is clear that enough has been done when these goals are achieved. In general, SKB has presented a detailed and well supported SDM that does represent sound science at the state-of-the-art. However, we did not identify how they are able to demonstrate that they have done enough. We have identified a number of unresolved questions, that may indeed not be significant in terms of the safety case, but by not setting out clear and quantified acceptance criteria for the models, it is hard to confirm that the modelling is complete for its purposes.
4. Parameterisation of DFN models and upscaling to ECPM. It was felt that a number of assumptions in the DFN modelling of the HRD were made, and alternatives were not clearly ruled out. For example T-S relations for the interference test models and fracture size-transmissivity relationships. The implementation of upscaling between Fracman and Darcytools appears appropriate, but this is an active research area and it is felt worthwhile to expand the scope of the review to investigate how this approach relates to other work on upscaling DFN models to ECPM. This is a very active research area in both nuclear and non-nuclear waste fields. It would also be

of interest to consider how else this has been addressed in the Swedish context by contrasting DFN versus ECPM model results in similar settings.

3

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Hydrogeological analysis in the safety assessment SR-PSU

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Abstract

The Swedish Nuclear Fuel and Waste Management Co. (SKB) has presented the safety assessment SR-PSU in support of a proposed extension of the SFR facility for low- and intermediate-level radioactive waste, located near Forsmark, Sweden. This report presents findings of an initial-phase review of hydrogeological analysis within SR-PSU.

Hydrogeological models are utilized directly in SR-PSU as the basis for calculating flows through the waste vaults and paths for radionuclide transport. They form the main basis for three key scenarios and play a role in seven additional scenarios involving degradation, breach, or omission of the engineered barriers.

The documentation of the hydrogeological analysis is sufficiently transparent for purposes of review. SKB's assessment model flowchart shows the main connections between hydrogeology and other models used in the safety assessment. Topics for more in-depth review have been identified based on consideration of the likely impact on the safety case.

An independent assessment of the uncertainties and simplifications in the hydrogeological site-descriptive model is recommended, with particular attention to the “high flow in bedrock” scenario. Key questions include the sufficiency of the limited set of variants and stochastic realizations that have been propagated to dose/risk calculations, for models of the hydraulic conductor domains (HCDs) and hydraulic rock domain (HRD). The flow models also appear to be sensitive to assumptions regarding the hydraulic properties of marine sediments and the sediment-bedrock interface.

SKB's treatment of concrete degradation processes and their impacts on flow does not directly account for heterogeneity – including fracturing – that would develop as the concrete barriers degrade; an interdisciplinary review of this topic is recommended. Estimates of the duration of the resaturation period are based on an old (2001) hydrogeological model model that differs in several key respects from the current site descriptive model; SKB's justifications for not modelling the resaturation period should therefore be examined. Additional review topics are identified regarding the “wells downstream of the repository” scenario, the earthquake scenario, and future human actions.

Contents

1. SKB’s presentation

The intent of this chapter is to give a preliminary assessment of the safety relevance of the review area, and to summarize the structure and identify the most relevant parts of SKB's documentation for hydrogeological review.

1.1. Safety relevance of review area

The SR-PSU main report (SKB, 2014a) provides a basis for assessing the safety relevance of hydrogeological analysis, by comparing the results of the following hydrogeology-related scenarios with the main scenario:

- High flow in bedrock,
- Wells downstream of the repository (Section 7.6.7),
- Intrusion wells (Section 7.6.8),

In addition the following scenarios consider situations where flows through one or more of the vaults can be enhanced by events or processes that lead to omission, breach or degradation of the engineered barriers:

- Accelerated concrete degradation (Section 7.6.3),
- Combination of accelerated concrete degradation with high flow in bedrock (Section 7.8),
- Bentonite degradation (Section 7.6.4),
- Earthquake (Section 7.6.5),
- Loss of barrier function – high water flow in repository (Section 7.7.3),
- Unclosed repository (Section 7.7.6),
- Future human actions (Section 7.7.7)

Hydrogeological aspects of these scenarios, and their impacts on safety according to SKB’s evaluation, are summarized in the subsections that follow. Figure 9-48 of the Main Report provides an overview of the relative consequences of these and other scenarios, in terms of the peak annual effective dose.

1.1.1. Main hydrogeological scenario

The main hydrogeological scenario is based on the interpretation of bedrock hydrogeology from the site-descriptive model (Öhman et al., 2012), as a component of SDM-PSU. This interpretation is the subject of a companion review (Geier, 2015). The interpretation is described in terms of the following main components:

- Hydraulic Conductor Domains (HCDs) representing hydraulically significant deformation zones,
- Hydraulic Rock Domains (HRDs) described in terms of a discrete-fracture network (DFN) model, and
- Shallow Bedrock Aquifer (SBA) structures to characterize high-transmissivity lateral connections in the shallow bedrock.

Estimated properties of the HCD, HRD, and SBA structures are provided in SKB R-11-03, which is used as starting point for SR-PSU hydrogeological modelling in SKB R-13-25. When the estimated properties of these components are used as a base case in the main hydrogeological scenario, the estimated dose to the most exposed group remains well within the bounds of the regulatory risk criterion.

1.1.2. High flow in bedrock scenario

The "high flow in bedrock" scenario (Main report, Section 7.6.2) uses hydrogeological data from a bedrock realization (bedrock case 11) that gives high flows relative to the realization (bedrock case 1) that was used for calculations in the main scenario. The differences between these cases are shown in terms of the median values of F_r and $t_{w,r}$ for each of the vaults as a function of time, in Figures 7-4 and 7-5 of the main report. The reduction of median F_r for the high-flow bedrock case is at most a factor of two, and generally less.

The detailed water flows inside the waste vaults for this scenario were constructed by a different approach, which is argued by SKB (2014a, p. 233) to be more conservative. Instead of using just the cross-flow values for a given vault from bedrock case 1, SKB has used ratios that represent the highest cross-flow for that vault, among all realizations of the bedrock model. SKB asserts that this is "non-physical" and hence overly conservative.

The outcome for this scenario (Main report, Section 9.3.2) indicates that it produces a modest, but significant increase in dose especially in the time interval from 3000 to 20,000 AD (Main Report, Figure 9-17). However even with this increase, the calculated doses are still only about half of the level corresponding to the risk criterion.

1.1.3. Wells downstream of the repository scenario

This scenario considers the possibility that future human inhabitants could drill wells downstream of the repository after the Baltic shoreline retreats beyond the repository footprint, and that these future inhabitants would then utilize water from these wells for domestic purposes. The assumptions of the scenario are explained in (Main report, Section 7.6.7).

A *well interaction area* is delineated in an area where there is a high density of flow pathways from the repository in future times. Based on an analysis by Werner et al. (2013), it is estimated that a well drawing from a depth interval of 10 m to 80 m below present-day ground surface could attract 10% of radionuclide discharge from the repository. The concentration of radionuclides in the well water is calculated by dividing the amount of radionuclides that are calculated to reach the well, but the amount of water that would be drawn from such a well for domestic use.

The risk contribution for this scenario is scaled by the probability of such a well being drilled in the well interaction area. This probability is calculated as the current density of wells in the Forsmark area (0.5 wells per km^2) times the well interaction area (about 0.26 km^2).

The results for this scenario are presented in Section 9.3.7 of the main report. For one category of exposed group (a garden plot household), the total dose comes close to this risk-equivalent dose from around 3500 AD to 5000 AD, at which point the risk criterion is briefly exceeded. For other types of exposed groups the dose remains well under the level that corresponds to the risk criterion.

According to the calculation of annual risk in Section 10.3.2, this scenario when added to the main scenario gives the highest maximum annual risk of any of the "less probable" scenarios.

1.1.4. Intrusion wells scenario

The *intrusion wells* scenario is described in Section 7.6.8 of the Main Report. This considers the possibility of a well for drinking water supply being drilled directly into the repository, sometime after the Baltic shoreline has retreated beyond the repository (3000 AD). The probability of such a well penetrating a given vault is estimated based on the current density of wells in the Forsmark area (0.5 wells per km^2) multiplied by the footprint area of each waste vault, and then multiplied by the fraction of current wells in the Forsmark area that reach the depth of the given waste vault.

The results as given in Section 9.3.8 of the Main Report show that for a garden-plot household, the annual dose resulting from using drinking water from such a well would exceed the dose corresponding to the risk criterion, for any of the vaults in the early period after 3000 AD, and for most vaults at least until 8000 AD. The exceptions are the BRT and the 1BLA, for which the dose drops off more rapidly. A supplementary calculation shows that the dose for 1BLA, which is initially very high in the base case, is sensitive to the transport properties of U-238, in combination with the flowrates in the 1BLA waste vault.

1.1.5. Accelerated concrete degradation

The *accelerated concrete degradation* scenario is described in Section 7.6.3 of the Main Report, which states that this scenario "assumes that the hydraulic conductivity of the concrete increases considerably earlier or to a greater extent than in the main scenario."

This scenario only affects the representation of the 1-2BMA and 1-2BTF vaults. For 1-2BMA, the difference with the main scenario is that the concrete is assumed to be severely degraded after 3000 AD (rather than 22,000 AD), and completely (rather than severely) degraded from 22,000 AD onward. For 1-2BTF, the concrete is assumed to go directly from "moderately degraded" to "completely degraded" after 3000 AD (rather than a transitional period of "severely degraded" from 3000 AD to 12,000 AD). Calculations of repository-scale flows for the different degradation states, for three different shoreline positions, are described in Section 6.2.1 of Abarca et al. (2013), but it is somewhat unclear how these calculations were utilised in the radionuclide transport and does calculations.

The outcome for this scenario (Main report, Section 9.3.3) indicates that it produces up a 50% increase in annual dose relative to the main (global warming) scenario, from 3000 AD when the accelerated degradation begins, with a peak dose 42% higher than the peak dose for the main scenario [Main Report Figure 9-23]. The calculated doses are not sufficient to exceed the risk criterion, but they approach within a factor of two.

The outcome of the scenario combining accelerated concrete degradation with high flow in bedrock is described in Section 9.5.1 of the Main Report. The peak annual dose for this scenario of 12.2 μSv, which approaches but still below the dose corresponding to the risk criterion.

1.1.6. Bentonite degradation

The *bentonite degradation* scenario is described in Section 7.6.4 of the Main Report. During the first permafrost period in the early periglacial climate case, an ice lens is assumed to form in the bentonite around the silo, resulting in a permanent increase in its hydraulic conductivity. The analysis of near-field flows is described in Section 6.2.4 of Abarca et al. (2013). The effects as described in Section 9.3.4 of the Main Report are minor in comparison with the accelerated concrete degradation scenario, with no significant increase in peak dose, though there is a slight increase in doses far into the future (after about 20,000 AD).

1.1.7. Earthquake

The earthquake scenario is described in Section 7.6.5 of the Main Report. The hydrological consequences are based on an assumption that the concrete barriers in the silo fail, so water flow increases. Results are discussed in Section 9.3.5. The peak dose for this scenario is at 4500 AD for an earthquake in 2100 AD, and is about three times as high as for the main (global warming) scenario. This is sufficient to exceed the dose corresponding to the risk criterion. However due to the method of calculating risk (weighting by the cumulative probability of an earthquake which increases monotonically with time), the peak risk occurs at a later date.

1.1.8. High water flow in repository

The loss of barrier function scenario involving high water flow in repository is considered as a “residual” scenario in Section 7.7.3 of the main report. The higher flows result from what SKB describes as an “unrealistic, pessimistic” assumption that all concrete and bentonite in the waste vaults and plugs have a hydraulic conductivity of 10^{-3} m/s. The analysis of near-field flows is described in Section 6.2.3 of Abarca et al. (2013). Porosities and diffusivities are based on the properties of degraded concrete. The results as presented in Section 9.4.3 of the Main Report show that the maximum dose increases by an order of magnitude, and exceeds the risk criterion. This demonstrates the importance of these barriers for long-term safety.

1.1.9. Unclosed repository

The case of an unclosed repository is considered as a “residual” scenario. The assumptions of this case are discussed in Section 7.7.6 of the Main Report, and is defined as calculation case CCR_UR in Section 8.5.6. Tunnels are left open and unsealed, and it is assumed that water from the tunnel entrance is used as drinking water, as the only exposure pathway. As presented in tabular form in Section 9.4.6, the peak doses are 3 to 4 orders of magnitude above the risk criterion, depending on the assumed inventory at the time of abandonment. Thus closure and sealing of the repository are essential for long-term safety of the repository.

1.1.10. Future human actions

Scenarios involving future human actions are discussed in Section 7.7.7. Actions discussed include:

- Drilling into the repository,
- Water management (removal or modifications to the SFR pier),
- Underground construction (tunnel or mine near repository),

Only the first of these is addressed quantitatively in Section 9.4.7. The quantitative treatment focuses on exposure of a drilling crew or future activities on a drilling detritus landfill, which does not have a close relationship to hydrological issues. The other two categories of actions are said to be addressed qualitatively in the FHA Report (SKB TR-14-08), which has not been reviewed for this task.

The handling of hydrological aspects of these potential future human actions could be a topic for the detailed review phase. One question, the answer to which is not obvious from the presentation in the Main Report, is whether the water management scenario includes the reasonable possibility that the SFR pier could be utilized and modified as part of a dam for a water impoundment.

1.2. Relevant documentation

The purpose of this section is to give a brief account of the structure and most relevant parts of SKB's documentation, in relation to the hydrogeological review area.

1.2.1. Safety assessment methodology

The safety assessment methodology is described in the Main Report, with an overview in Chapter 2 and discussion of the handling of features, events, and processes (FEPs) in Chapter 3. This review has not focused on broad methodological issues so these sections were used just as background information.

1.2.2. Initial state

The initial state of the repository is primarily described in the Initial State report (SKB TR-14-02). This describes the initial state of the proposed extended SFR, including various aspects of the waste (types, packaging, and acceptance criteria), design features and main dimensions of the different vaults, allocation of waste packages to different vaults, material quantities, radionuclide inventories, and inspection/control procedures.

This review focused on Chapter 12, but some other chapters could be useful as information for a more detailed review of hydrogeological processes in and around the SFR. Specifically Section 3.6 describes the waste packaging, including concrete moulds and concrete tanks for which the permeability of the packaging could be a factor for considerations. Section 3.7 describes the distribution of waste among the different vaults. Chapters 4 through 10 describe the design and type of waste and waste packaging planned for storage in each of the different types of vaults. Chapter 11 describes plugs and other closure components, and thus may be relevant for assessing the realism of the hydrogeological models that take account of these components.

In Chapter 12, this review has focused on the subsections that relate to hydrogeological variables. Subsections 12.1.4 (waste form), 12.2.3 (waste packaging), 12.3.3 (1BMA and 2BMA components), 12.5.3 (silo system components), and 12.6.3 (1BLA and 2-5BLA components) all refer repetitively to an early modelling study (Holmén and Stigsson, 2001) as the source of an estimate of 25 years for resaturation. Sections 12.4.3 (1BTF and 2BTF components) and 12.6.3 (BRT components) avoid this repetition by referring to 12.3.3.

1.2.3. Processes

Processes considered in this review are discussed in terms of the following main categories:

- Waste forms and waste packaging processes,
- Engineered-barrier processes,
- Geosphere processes.

These are discussed sequentially in the paragraphs below.

Waste forms and waste packaging

SKB TR-14-03 (Sections 3.3 and 4.2 considered here) is a high-level discussion of processes affecting and affected by the waste forms and packaging. An inventory of processes and interactions is given, mainly in qualitative terms. TR-14-03 Section 3.3 (p. 45) discusses resaturation of repository components.

In SKB TR-14-03 Section 3.3.1, mechanisms for dissipation of air from the different porous materials are discussed, including: (1) flow of air as a gas phase in dry pores or as bubbles, (2) dissolution of gas into water, possibly limited by solubility and transport by diffusion and/or advective flow of water, and (3) by reactions that consume component gases such as oxygen. The rate at which these processes occur may delay saturation.

Engineered-barrier processes

SKB TR-14-04 (Sections 5.2, 6.2, 7.2, 8.2, 9.2, and 10.2 considered here) is a high-level discussion of processes affecting and affected by the engineered barriers. As with the corresponding report for waste and waste packaging, the inventory of processes and interactions is given mainly in qualitative terms. The range of physical and chemical processes considered is reasonably comprehensive for the type of facility and expected hydrogeological conditions during operation and after closure.

Geosphere processes

SKB TR-14-05 is aimed to describe the current scientific understanding of the processes in the geosphere that are potentially relevant for long-term safety of the repository, and to explain why each identified process is handled in a particular way in the safety assessment. Chapter 3 is the main chapter covering hydraulic processes in the geosphere, with separate sections on groundwater flow and gas flow/dissolution.

Other geosphere processes that could affect groundwater flow include:

- heat transport (Section 2.1),
- freezing in periglacial conditions (Section 2.2),
- displacement along existing fractures (Section 4.3),
- fracturing (Section 4.4),
- erosion and sedimentation in fractures (Section 4.5),
- dissolution/precipitation of fracture-filling minerals (Section 5.6), and
- degradation of grout (Section 5.8).

The description of groundwater flow in the geosphere process report (SKB TR-14-05, Section 3.1), is brief and at a general level. Reference is given to the corresponding report for SR-Site, as a more comprehensive description.

1.2.4. Models and data

Models relevant for hydrogeological/hydrological analysis

The main numerical software used in SR-PSU is documented in SKB TR-14-11. For each code, the report discusses the suitability of the code, its usage in SR-PSU, its development process and verification, the handling of input data and results, and the rationale for using the code in the assessment. The codes of most direct concern for hydrogeology and surface hydrology are Comsol Multiphysics (used for near-field hydrological calculations, Section 3.5), DarcyTools (used for bedrock hydrogeological calculations, section 3.6), Ecolego (used for radionuclide transport calculations, Section 3.7), and MIKE SHE (used for near-surface hydrogeology and surface hydrology, Section 3.9).

Of these, all except DarcyTools are considered by SKB to be widely used commercial codes. DarcyTools has only been used in SKB projects. It is noted in Section 3.6.4 that “no attempt has been made to show that DarcyTools conforms to any international QA standard.” As noted in 3.6.3, DarcyTools includes a FORTRAN input file which allows implementation of advanced features that can go beyond the compiled form of the program. These include transient boundary conditions and source/sink terms. To the extent that these features have been used in SR-PSU, it should be considered that the application may extend beyond the types of verification that has been performed. The rationale for using this code is stated in Section 3.6.6 of SKB TR-14-11 to be “because it has been developed by [SKB's consultants] in cooperation with SKB especially for solving the problem at hand.”

Codes of indirect interest for hydrology include ArcGIS (used for terrain, regolith, and landscape development models), a Glacial Isostatic Adjustment code (used to calculate relative sea level and shoreline migration which determine boundary conditions for future hydrology), a numerical permafrost model (used to calculate the timing and extent of permafrost which affects upper boundary conditions and permeabilities), and a numerical ice-sheet model (used for calculating ice sheet advance and retreat which affects upper boundary conditions as well as permafrost conditions.

Inputs to hydrogeological/hydrological analysis

The Assessment Model Flowchart (AMF) given in Appendix B of SKB TR-14-12 documents the flow of data between models. The main inputs to hydrogeology according to the AMF are:

- Landscape modelling (AMF 1),
- Site-specific model for bedrock hydrogeology (AMF 4), and
- Climate cases (AMF 18),

where the numbers refer to input/output data items on the AMF. Landscape model inputs (AMF 1) are documented in Section 6.1 of SKB-TR-14-12 and include geometrical data for the bedrock and regolith, development of lakes and streams, and location of future taliks. The site-specific model for bedrock hydrogeology (AMF 4) is taken from SDM-PSU, which is the subject of a separate review (Geier, 2015). Properties of the HCD, SBA, and HRD are taken to be as prescribed in the hydrogeological site descriptive model (SKB R-11-03; see also see Section 1.1.1) which is used as starting point for SR-PSU hydrogeological modelling in SKB R-13-25. The climate data referenced for AMF 18 are the maximum permafrost depth and the shoreline evolution, are documented in Section 5.2 of SKB-TR-14-12, which refers to specific sections of the Climate report for further details as well as additional documents.

Inputs to near-field hydrology include (in addition to hydrogeology, AMF 7) are:

- Evolution of concrete barriers (AMF 45),

- Evolution of bentonite barriers and plugs (AMF 46),
- Repository layout/geometries (AMF 127)

From the description of the hydrogeological modelling for SR-PLU (Öhman et al., 2013), evidently the repository geometry and hydraulic properties of the concrete and bentonite barriers are also used as input for hydrogeological modelling, but this data transfer is not shown on the AMF.

Data on well locations, depths and yields (AMF 172) are used as input to modelling of wells in the repository discharge area.

Hydrogeological inputs to safety analysis

The different hydrogeological calculations are used for multiple purposes in the subsequent safety analysis steps. According to SKB R-13-25, p. 12, hydrogeological modelling for SR-PSU serve the following main purposes:

- Descriptions of hydrogeological conditions during temperate and periglacial climate conditions;
- Results exported to other disciplines (RN transport, hydrogeochemistry, and biosphere analyses).

Particular attention is given to climate- and surface-system-driven evolution of hydrogeological conditions, including changes from discharge to recharge circumstances for a given area.

The key performance measures listed in R-13-25 (p. 81) are:

- Disposal room cross flows;
- Exit locations at the bedrock/regolith interface,
- Flow-related transport resistances in the bedrock along pathways determined by particle tracking, and
- Advective travel times in the bedrock along pathways determined by particle tracking.

An additional performance measure of “supporting character” is:

- Path lengths in the bedrock along pathways determined by particle tracking.

The major uses of hydrogeological data are detailed in the Assessment Model Flowchart (TR-14-12 Appendix B) and in the text of the same report.

Hydrogeological model outputs used as input to the near-field hydrological model of Abarca et al. (2013) are documented as AMF 7 in Section 4.5 of TR-14-12. These comprise (1) the pressure at the SFR rock volume boundaries, (2) groundwater velocities in the bedrock at the SFR location, and (3) the calculated anisotropic hydraulic conductivity of the bedrock.

Particle trajectories calculated with the DarcyTools model (AMF 9) are used as input to the models of geochemical evolution

F-factors and travel times for travel paths from each vault to the surface (AMF 11) are used as input to the Ecolego models for radionuclide transport in the water phase.

The Peclet number used for the entire rock volume (also part of AMF 11) was not derived from hydrogeological modelling for SR-PLU, but simply taken from SKB's 2001 SR-SAFE, according to Section 4.8.3 of SKB TR-14-12. Peclet number is also listed as AMF 211, and according to Section 4.27 of the same report this is taken from SKB's 2010 SR-Site safety assessment. Both of these are shown as input to the Ecolego models for radionuclide transport in the water phase, according to the AMF.

Hydrogeological model outputs used for RN transport (water phase) calculations are:

- Exit locations coordinates) for defined time steps/events (AMF 11),
- Well-related flow data – dose to well (AMF 136).

Hydrogeological model outputs used for biosphere modelling (input to dose calculations) are:

- Biosphere object identification – exit locations (AMF 12),
- Inputs to surface hydrology – hydraulic conductivities (AMF 84).

These data furnished are described in Sections 4.9 and 4.17 of SKB TR-14-12; links to the datasets are given but apparently require a security code to access.

The linkage between hydrogeological models and concrete-barrier evolution models appears to be circular (or iterative) according to the AMF:

- Water flow and flow patterns within the vaults, backfill, and concrete barriers based on near-field hydrogeology models (AMF 153) are shown as an input to models for rebar corrosion and degradation of concrete,
- Results of the rebar corrosion and concrete-degradation models in terms of the impact of chemical processes on concrete (AMF 38) are used as input for models of the evolution of concrete degradation, and
- Porosities and hydraulic conductivities of concrete materials in SFR based on models for the evolution of concrete degradation (AMF 46) are used as input for near-field hydrogeology models.

In contrast to the models of concrete-barrier evolution, the AMF does not show any inputs from near-field hydrogeology to the models of bentonite-barrier and plug evolution, although the latter feed into near-field hydrogeology (via AMF 46). Specifically, the AMF does not show any influence of near-field hydrogeology on bentonite barriers via mechanisms such as bentonite erosion.

The only inputs to bentonite-barrier and plug evolution models, according to the AMF, are calculations of permafrost depth (AMF 74) and an assessment of ice-lens formation in the silo (AMF 185) which feed into calculations of bentonite freezing, plus bentonite/plug initial state and material properties (AMFs 205 and 44). Site-specific hydrogeological properties might enter into the calculations of permafrost depth as input to models of climate cases, representing prolonged interglacial conditions, which are used for the permafrost depth calculations (AMF 74).

1.2.5. Hydrological modelling

Surface hydrology and shallow hydrogeology

R-13-19 (Werner et al. 2013) provides modelling results and descriptions of present and future hydrological and near-surface hydrogeological conditions at Forsmark. The modelling is performed using the MIKE SHE software, as for the equivalent modelling in SR-Site. Results are presented for both present-day temperate and future permafrost/periglacial conditions in terms of water balance, vertical hydraulic head differences between the regolith and the bedrock, depth to the groundwater table, depth of overland water and stream discharge, residence times and inter-basin water exchanges of marine basins. The results for different discharge locations are related to biosphere objects.

Chapter 6 of R-13-19 considers water resources management and exploitation by future inhabitants of the Forsmark area, considering the potential water supplies and capture zones of potential wells, including wells in bedrock. Particle tracking making use of the DarcyTools code is used to investigate the potential for flow to a well to draw in contaminated water for an exposed group farming or growing vegetables in the area. Probability of intrusion of a well is also considered. Thus this report deals with human intrusion issues as well as predictions for the main scenarios.

Flow modelling on the repository scale

SKB TR-13-08 (Abarca et al., 2013) presents deterministic modelling of flow through the engineered barriers in the repository, using heterogeneous hydraulic conductivity fields extracted from the DarcyTools model of Odén et al. (2014). Boundary conditions for the near-field flow model are also extracted from DarcyTools. Calculations are carried out for a base case (in terms of hydraulic properties) considering three different shoreline positions, then for various cases of barrier/plug degradation and formation of an ice lens in the Silo. Two different closure alternatives are considered, as well as the case of an abandoned, open repository, and a shallow permafrost case. Finally uncertainties associated with the geosphere are calculated.

Far-field hydrogeological modelling

The hydrogeological modelling for SR-PSU is described by Odén et al (2014; SKB TR-13-25), as a top-level report. Further details of the calculations are given in three progress reports: SKB P-14-04, P-14-05, and P-14-06, as described in the following paragraphs.

SKB P-14-04 (Öhman et al., 2014) covers the main hydrogeological calculations for the temperate periods. It assesses the combined effects of bedrock heterogeneity, parameterisation uncertainty, and transient flow regime in terms of performance measures. A sensitivity analysis is carried out by considering 17 “Bedrock” cases (different hydraulic parameterisations of the bedrock) in combination with six selected stages of shoreline retreat. The main results are in terms of quantitative performance measures for SR-PSU:

- Disposal-room cross flow, Q (m^3/s),
- Coordinates of particle exit locations at the bedrock/regolith interface,
- Flow-related transport resistance along bedrock flow paths, F_r (y/m), and
- Advective travel times along bedrock flow paths, $t_{w,r}$ (y).

SKB P-14-05 (Öhman and Vidstrand, 2014) focuses on interactions between the SFR facilities and potential future water-supply wells in the area. Water-supply wells are considered both for settlements associated with areas that are predicted to have arable land after shoreline retreat according to Werner et al. (2013), and for the "well-interaction area" which has the highest concentrations of radionuclides originating from the repository based on particle-tracking results for the temperate period. The analyses consider both the effect of the wells on flows through the waste vaults in the SFR, and the fraction of well discharge that is drawn from the repository. Wells in the future arable areas are indicated to have very little interaction with flows through the repository. The results for wells in the "well-interaction area" are used in the assessment of the downstream wells scenario.

SKB P-14-06 (Vidstrand et al., 2014) describes hydrogeological calculations for future periglacial periods. The model uses the same bedrock model as for the temperate case, but with thermally/hydraulically coupled solutions for flow and heat transport. Similar to the temperate model, the main results are in terms of quantitative performance measures for SR-PSU:

- Disposal-room through-flows (total and local values),
- Exit locations for particle traces passing through repository vaults an through the bedrock to the bedrock/regolith interface, and
- Darcy fluxes, flow-related transport resistance, path lengths and travel times along bedrock flow paths

The pressure field in the near-field of the SFR is also calculated as input to the near-field flow modelling. Permafrost is studied by means of two variants: One in which the frozen ground reaches elevations just above SFR 1, and one in which frozen ground reaches elevations between SFR 1 and the SFR 3. Results are delivered for combinations of three different bedrock cases, three different permafrost depths, and three different landscape variants.

1.2.6. Hydrogeological uncertainties

Hydrogeological uncertainties identified in the site-descriptive modelling phase are summarized in Sections 7.6 and 9.8 of SKB TR-11-04:

1. Parameterisation uncertainty for regolith layers, especially the offshore marine sediments which control flow between sea and bedrock;
2. Uncertainty in parameterization of steeply dipping deformation zones;
3. Occurrence and size, nature and transmissivity of hydraulically significant sub-horizontal to gently dipping small-scale structures (minor deformation zones and discrete fractures) in shallow bedrock;
4. Occurrence of high PFL-f transmissivities outside of the deterministic deformation zones, leading to speculation of insufficient borehole coverage

and a need for sensitivity studies if no more boreholes are drilled to investigate these areas (TR-11-04, p. 236).

5. Apparent compartmentalization of flow system in gently dipping features in shallow bedrock due to heterogeneity and/or other factors (not stated explicitly by the authors but presumably channelling is one possibility);
6. Variable quality of historical data support;
7. Conceptual questions about the reasons for systematically lower transmissivity as interpreted from Posiva Flow Log anomalies (PFL-f) inside the central block compared with closer to the Southern and Northern Boundary belts.
8. Uncertainty in Hydro-DFN model due to censoring related to the practical detection limit of the PFL-f method.
9. Decreasing borehole sample size with depth, which affects estimates of trends in transmissivity with depth;
10. Limited sample size for parameterization of Shallow and Deep domains of HRD.
11. Lack of clear understanding of reason for decreasing inflow in tunnels, though several hypotheses are viable and imply reversibility of this effect after closure;
12. Uncertain measurements of inflow data due to ventilation system.

Issue (2) is also brought up in a list of recommended model variants.

1.2.7. Use of results from hydrological modelling

Radionuclide transport and dose calculations are described in SKB TR-14-09 (Table 4-17 summarizes calculation cases). The relationship of the hydrogeological and hydrological models to these calculations for the main scenario is via a set of 100 “iterations” for the near-field model and far-field model based on Monte Carlo simulations with Latin hypercube sampling. Each of these is then combined with 10 realizations of input parameters for the biosphere model.

The near-field and far-field models are compartment models, implemented in Ecolego. The connection of these models to the hydrological modelling is illustration in Figure 1.

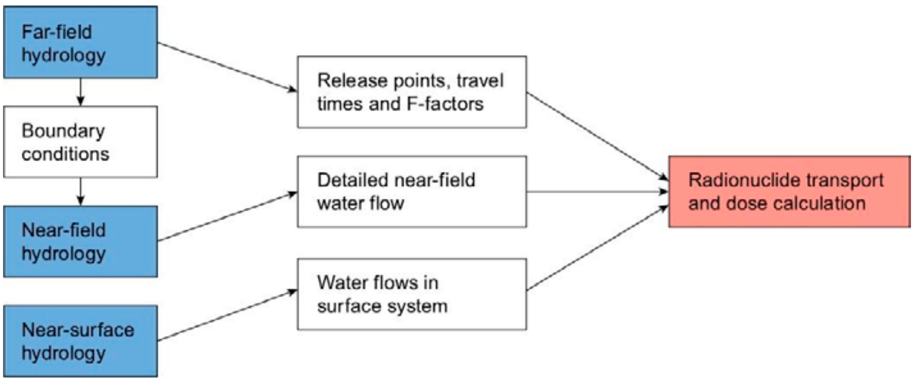

Figure 1: Conceptual diagram of data transferred from hydrological models to radionuclide transport and dose calculations (from SKB TR-14-09, Figure 9-1).

The compartment models for the near field are described in described in Section 8.2.3 of SKB TR-14-01 and with additional details in Section 9.3 of SKB TR-14-09. Flowrate data from the COMSOL model to Ecolego are in terms of annual flows between control volumes defined by Abarca et al. (2013). Each control volume is represented by a single compartment or a group of compartments.

The compartment model for the far field is described briefly in Section 8.2.4 of SKB TR-14-01. Further details are given in Section 9.4 of TR-14-09. Groundwater flow fields are stated to be taken from the DarcyTools hydrogeological model (Odén et al., 2014).

Biosphere models are discussed in Section 9.5 of SKB TR-14-09. According to Section 9.5.1 the locations of discharge areas are based on hydrogeological modeling by Odén et al. (2014).

2. Assessment of SKB's presentation

2.1. Overall quality of documentation

2.1.1. Structure and transparency

The hydrogeological and surface hydrological modelling reports are generally well structured and are reasonably transparent, particularly in explaining what combinations of variants were considered, and how these are defined. The tables of terminology and acronyms (for example Table 1-4 of SKB TR-11-10 and Table 1-2 of SKB TR-13-25) are especially helpful. Conceptual assumptions, input data, boundary conditions, and key output data are reasonably well explained, using an appropriate report structure for the purpose.

One weakness is that the main numerical model used for the deep hydrogeological system, DarcyTools, is explained only briefly as a series of equations solved, for example in Appendix A of SKB TR-13-25), and a very general summary in the Models summary report. A thorough discussion is lacking of the capabilities of this model in terms of its reliability and sensitivity for the types of calculations undertaken.

References are given to the user documentation, code description and verification documentation for Darcy Tools Version 3.4 (Svensson and Ferry, 2010; Svensson et al., 2010; Svensson, 2010), which could be used as the basis for a more in-depth review. However in the background report SKB P-14-04, Section 2.1.1 it is stated that DarcyTools Version 3.4.18 was used in combination with Migal Version 4.01 (the latter not explained), and that an error was found in a pressure-correction algorithm, which is explained only in qualitative terms. Reference is given to SKBdoc 1396127 as an explanation of the error and the workaround that was employed. Thus it could be relevant for review to ascertain if the version of DarcyTools that was used is fully explained by the 2010 documentation.

The process reports for the waste forms, waste packaging and engineered barriers (SKB TR-14-03 and TR-14-04) are unnecessarily bulky and repetitive, due to the chosen structure in which all processes are discussed (or at least represented by section headings) for each of the five categories of vaults, and again for the plugs and closure components. An attempt has been made to reduce the degree of redundancy by use of cross-references, but the way in which this is done is inconsistent. For example the first paragraph under the heading "Matrix flow" in Section 7.2.1 of SKB TR-14-04 is repeated verbatim from the corresponding heading of Section 5.2.1, before giving a cross-reference to Sections 5.2.1 and 5.2.2. A more efficient, transparent and consistent structure could have been based on identifying the key processes in the main types of materials (concrete, bentonite, etc.) and then simply noting which of these apply for different vaults, and how the details of design affect their interactions.

As one example of the awkwardness produced by this structure, in Section 5.2.2 of SKB TR-14-04 the discussion of water transport under saturated conditions in the BMA (where concrete is stated to be the most important barrier) lists references that appear to refer to clay (Dixon et al., 1999; Hansbo, 1960) as examples of deviations from Darcy's Law.

The presentations of unsaturated flow and saturated flow in Sections 5.2, 6.2, …, 10.2 of SKB TR-14-04, are in order of the expected occurrence of the processes after closure, rather than proceeding from the simpler process (saturated flow) to the more complicated process (unsaturated flow). This leads to an unwieldy presentation in which a pedagogical but very wide-ranging discussion of the physical processes of unsaturated flow appears first, then a brief description of saturated flow states that this is a simpler case of unsaturated flow.

The paragraph regarding the "adequacy of references supporting the handling in SR-PSU" is identical in nearly all of the 30 sections of SKB TR-14-04 where it appears:

> *"The references are judged to be adequate and sufficient to support the handling in SR-PSU. All supporting references are either peer-reviewed articles or documents which have undergone factual review. Other references have been used for general background information, and not all of these have been peer-reviewed to the same standard."*

This paragraph gives little information, as there is no explanation of which of the cited references are regarded as "supporting" references versus those that were used for background information. The repetitive use of "boilerplate" paragraphs such as this erodes confidence in the thoroughness of the safety assessment; the impression is that this was just a matter of checking off boxes, with no serious attempt to analyse or otherwise evaluate the particular topic.

As an example at the other extreme, the cross-reference to Section 5.2.2 in the paragraph "Natural analogues/observations in nature" in Section 10.2.2 of SKB TR-14-04 refers to just a single sentence of limited relevance and specificity. This type of cross-reference also raises doubts about the thoroughness of SKB's analysis.

The standard implied by the term "factual review" is unclear. Reports from SKB-sponsored research from decades past are cited along with much more recent reports that were used directly as supporting evidence for SR-Site. Should all of these be judged as equivalent in terms of the level of factual review?

The very brief comments under the headings, "Natural analogues/observations in nature" in SKB TR-14-04 are perfunctory and uninformative. In several cases natural analogues are dismissed on the grounds that the engineering designs of components in the vault are unlike situations found in nature. This narrow approach fails to consider natural analogues that might apply to key components (such as hydrologic features of naturally occurring bentonite deposits) even if not the entire design. Archaeological analogues are not discussed. Section 5.2.2 mentions "water tightness of concrete structures" as a possible analogue (though "not strictly applicable," apparently because these are not "natural"), but does not discuss any specific cases or the lessons that might be drawn, e.g. from the long-term hydrologic behaviour of concrete structures from the Roman Empire. Overall the impression gained is that little serious effort has been given to identifying natural or archaeological analogues, and elucidating whatever safety-relevant lessons could be drawn from these.

2.1.2. Traceability

The Assessment Model Flowchart (AMF) given in Appendix B of SKB TR-14-12 provides a useful map of the data flow between models. The input/output data transfers are numbered as “AMF 1,” “AMF 2” etc. on this chart and can be checked by comparing to the corresponding AFM Number items in the text. The usefulness of this report for traceability is hindered by the fact that the different AMF items are not listed sequentially. A sequential index, or else an electronic version of the AMF with hyperlinks to the explanatory text, could be useful for the detailed review phase.

For many of the data items in SKB TR-14-12, web links are given to the datasets that were transferred between models. Attempts to access these links, as part of this review, led to an SKB web page that requires “authentication” for further access. Thus access to these links will need to be requested for future stages of the SR-PSU review. From a positive perspective, these links, once accessible, could obviate the need for numerous requests for complementary information that could be satisfied by access to detailed datasets.

Some gaps and inconsistencies in the AMF were noted. For example, from the description of the hydrogeological modelling for SR-PSU (Öhman et al., 2013), evidently the repository geometry and hydraulic properties of the concrete and bentonite barriers are also used as input for hydrogeological modelling, but this data transfer is not shown on the AMF.

The Peclet number used for the entire rock volume (also part of AMF 11) was not derived from hydrogeological modelling for SR-PSU, but simply taken from SKB’s 2001 SR-SAFE, according to Section 4.8.3 of SKB TR-14-12. Peclet number is also listed as AMF 211, and according to Section 4.27 of the same report this is taken from SKB’s 2010 SR-Site safety assessment. Both of these are shown as input to the Ecolego models for radionuclide transport in the water phase, according to the AMF, so this is confusing and raises a question of consistency.

The compartment model for the far field is described only briefly in Section 8.2.4 of SKB TR-14-01, with some further details given in Section 9.4 of TR-14-09. Groundwater flow fields are said to be taken from the DarcyTools hydrogeological model (Odén et al., 2014), but the specific parameters extracted are not clear from this presentation. Also not clear is whether dispersion parameters are estimated from particle-tracking in the flow model, or by some other means.

In the discussion of biosphere models in Section 9.5.1 of SKB TR-14-09, the locations of discharge areas are based on hydrogeological modeling by Odén et al. (2014), but no further details are given there as to how the output data from the hydrogeological models are used, or related to the shallow/surface water modeling by Werner et al. (2013). Possibly the Biosphere synthesis report (not reviewed here) mentioned on p. 206 gives more explicit information. Appendix A of SKB TR-14-09 gives just three brief paragraphs on p. 226 to describe the transfer of data from the tasks described by Odén et al. (2013) to Ecolego, plus plots of travel time and flow wetted surface area distributions (According to SKB TR-14-09, p. 205, flow wetted surface is calculated from the F-factor, so the latter seems to be the parameter that was transferred between models). The main data exchange was as text files for each of 100,000 particle tracks. Possibly these data should be requested for SSM's further analysis of dispersion, pathway properties etc.

2.1.3. Scientific soundness

In most respects, the hydrogeological safety arguments advanced by SKB are scientifically sound and are supported by substantial research. A few exceptions are noted below, but these should not be viewed as detracting from the overall result.

In introducing the *intrusion wells* scenario (Section 7.6.8 of the Main Report, p. 237), SKB suggests that, since the repository is deeper than the typical depth of water supply wells in the Forsmark area (about 60 m per Werner et al., 2014), it is conservative to assume that the well is assumed to fully penetrate a given waste vault. However from the calculation of probability described in the same paragraph, it can be seen that this is taken into account in a realistic rather than conservative way.

The description of groundwater flow in the geosphere process report SKB TR-14-05, Section 3.1 refers to the corresponding report for SR-Site, as a more comprehensive description. In discussing the role of bedrock structures, reference is made to Werner et al. (2007, SKB R-07-08) which was a study of recharge/discharge classification methods for shallow groundwater. It is surprising that no mention is made of SKB's model of superregional flow in northern Uppland (Holmén et al., 2003) which considered deep groundwater flow, for a region that includes the SFR site.

Seasonal fluctuations in groundwater levels are not modelled as part of SR-PSU (SKB TR-14-05, p. 60). Considering the shallow depth of the facility, there should be an evaluation of whether seasonal fluctuations contribute significantly to dispersion in the far-field. A more detailed review of this issue could be based on seasonal head changes for terrestrial parts of the investigated area.

Groundwater flow in SR-PSU is modelled as flow through an equivalent continuum porous medium (ECPM) based on upscaling from a stochastic DFN model and the deformation zones assessed in SDM-PSU (SKB TR-14-05, p. 60). Channelized flow within fractures is not considered (SKB TR-14-05, p. 63) either in the analysis of data to derive the DFN model, or in the upscaling.

The description of gas flow/dissolution processes in SKB TR-14-05, Section 3.3 is brief and of a general nature: “Detailed modelling of gas migration in fracture networks of the type of rock that hosts SFR has not been reported in the open literature.” Is this factual, or just an example of inadequate search of the relevant literature? However, the line of argument is reasonable, that the instabilities of gas flow in a partly water-filled fracture network would make explicit modeling of this process very complex, especially lacking detailed knowledge of fracture channel geometry.

The approach stated on p. 64 of SKB TR-14-05 is to assume that gas residence time is so short that the generated gas immediately reaches the biosphere and deposits any transported radionuclides there. With this assumption, the only limiting processes are the rate of gas generation (discussed on p. 66), its flow through the waste containers and engineered barriers (discussed on p. 67 somewhat inappropriately as this process should be dealt with in SKB TR-14-03 and SKB TR-14-04), and mechanisms for entrainment of radionuclides in the gas flow.

One weakness of neglecting the mechanisms of gas transport is that this approach limits the basis for discussion of radionuclide transport by attachment to gas bubbles. SKB TR-14-05 Section 3.3 gives a cross-reference to Section 6.3, where this mechanism is discussed (p. 236) as a “scenario” in which gas is produced by corrosion of metal parts, but the effects are judged to be marginal (p. 239). These arguments appear to be based on qualitative reasoning rather than quantitative assessments, at least in the sections of the report considered in this review. Further review of the potential for gas bubbles to play a role in transport could be warranted.

2.2. Adequacy of models, data and safety functions

2.2.1. Hydraulic properties of engineered components

In the Initial State report (SKB TR-14-02), hydraulic conductivity of the waste forms is discussed only in qualitative terms (“very permeable to almost completely tight”) in Section 12.1.4, but no data are given. Section 12.2.3 states that hydraulic conductivity data for the different concrete types can be found in the Data report (SKB TR-14-10). Section 12.3.3 likewise refers to the Data report regarding concrete structures in the BMA vaults. Here it is also noted that the hydraulic conductivity of macadam is “high, initially higher than 10^{-2} m/s (SKBdoc 1358612). For the silo, Section 12.5.3 gives hydraulic conductivity values for the bentonite used as wall fill (noting a range from $9x10^{-12}$ m/s in the lower part to $9x10^{-11}$ m/s in the upper part due to gravitational self-compaction) and for the sand-bentonite mixture in the top and bottom (less than $1x10^{-9}$ m/s). A report by Pusch (2003) is listed as the source of these values.

For the plugs and other concrete closure components, Section 12.8.3 of SKB TR-14-02 states that the hydraulic conductivity is “assumed to be the same as assumed for the concrete plugs in the BMA vaults,” with reference to the Data report. SKB doc 1358612 is again cited for the hydraulic conductivity of macadam. For bentonite in the connecting tunnels, a value of less than 10^{-10} m/s is assumed based on the value used for deposition tunnels in the spent-fuel repository (SKB, 2010, p. 151). The value of hydraulic conductivity for access tunnels is “calculated” based on a design requirement for flow resistance, rather than being based on measurements.

The hydrological consequences of fracturing of the waste, waste packaging and/or concrete barriers (mentioned in Sections 12.1.5, 12.2.4, and 12.3.4) are not discussed. The likelihood of rapid and extensive hydrogen production by corrosion of aluminium after saturation is mentioned in Section 12.1.9.

2.2.2. Resaturation processes

The presentation of physical and chemical resaturation processes in SKB TR-03 is reasonably comprehensive for the type of facility and expected hydrogeological conditions during operation and after closure. The discussion of processes that need to be considered in the analysis is also generally well-reasoned.

The decision not to model the resaturation period is supported in Section 3.3.7 by reference to modeling studies (Painter and Sun, 2005; Svensson and Follin, 2010). The brief arguments given under the heading “Excavation/operation/re-saturation period” on p. 73 are more pertinent to groundwater flow than to gas flow, and should have been part of Section 3.2. These additional references should be considered as a more detailed review of the potential significance of the resaturation period.

It is not clear that the processes that constrain dissipation of air from porous materials in the repository have been accounted for in the calculations of the 25-year saturation period by Holmén and Stigsson (2001).

Carbonatisation during the operational phase is mentioned in TR-14-03, p. 41 as a process that might affect the hydraulic properties of the concrete materials in the SFR, "to some degree." It is not clear from the documentation considered here, whether this issue has been analysed as part of the safety assessment, or what effects are anticipated as a consequence. Could these effects include development of heterogeneity within the concrete that is not accounted for in the models?

2.2.3. Influence of fracturing on flow

In the discussion of influence of mechanical processes on water uptake and saturation in waste forms and containers in TR-14-03 Sections 3.3.1 and 4.2.1, the potential for fracturing is not mentioned. Presumably fracturing of the concrete components and/or waste forms could help to accelerate saturation by providing paths for advective flow of water and gas migration by bubble flow. Fracturing caused by mechanical stress is mentioned as a factor for water uptake and transport under saturated conditions (Sections 3.3.2 and 4.2.2).

In Section 3.4 which discusses mechanical processes in the waste, SKB states that "the majority of fracture-generating processes are expected to occur post-closure." This might justify ignoring fractures in the resaturation stage, but the relative time frames for resaturation and fracture-generating processes are not discussed. The role of fractures for hydrological variables with regard to the waste form is discussed only briefly on p. 53, where SKB states, "The extent and connectivity of fractures will influence the flow pattern in the repository. However flow patterns will only be affected at a late stage when the outer barriers and packaging have failed."

A more thorough discussion of the hydrological consequences of fracture-generating processes in the waste containers and engineered barriers is warranted, and could be a subject for a request for complementary information.

2.3. Handling of uncertainties

The hydrogeological uncertainties identified by SKB in the site-descriptive modelling phase (Sections 7.6 and 9.8 of SKB TR-11-04) as listed in Section 1.2.6 are re-stated here:

1. Parameterisation uncertainty for regolith layers, especially the offshore marine sediments which control flow between sea and bedrock;
2. Uncertainty in parameterization of steeply dipping deformation zones;
3. Occurrence and size, nature and transmissivity of hydraulically significant sub-horizontal to gently dipping small-scale structures (minor deformation zones and discrete fractures) in shallow bedrock;
4. Occurrence of high PFL-f transmissivities outside of the deterministic deformation zones, leading to speculation of insufficient borehole coverage and a need for sensitivity studies if no more boreholes are drilled to investigate these areas (TR-11-04, p. 236).

5. Apparent compartmentalization of flow system in gently dipping features in shallow bedrock due to heterogeneity and/or other factors (not stated explicitly by the authors but presumably channelling is one possibility);
6. Variable quality of historical data support;
7. Conceptual questions about the reasons for systematically lower transmissivity as interpreted from Posiva Flow Log anomalies (PFL-f) inside the central block compared with closer to the Southern and Northern Boundary belts.
8. Uncertainty in Hydro-DFN model due to censoring related to the practical detection limit of the PFL-f method.
9. Decreasing borehole sample size with depth, which affects estimates of trends in transmissivity with depth;
10. Limited sample size for parameterization of Shallow and Deep domains of HRD.
11. Lack of clear understanding of reason for decreasing inflow in tunnels, though several hypotheses are viable and imply reversibility of this effect after closure;
12. Uncertain measurements of inflow data due to ventilation system.

Issue (2) is brought up in a list of recommended model variants, the handling of which in SR-PSU is discussed in Section 2.3.1. Issues involving the limitations of historical data (6) cannot be remedied and must simply be acknowledged. The remaining issues are discussed sequentially in the subsequent sections.

2.3.1. Handling of model variants recommended in SDM-PSU

In Section 9.9.2 of SKB TR-11-04, four specific types of model variants are suggested to address the key uncertainties:

1. Variants with different models for depth dependence and heterogeneity of transmissivity in the steeply dipping HCDs;
2. A variant in which the gently dipping deformation zone ZFM871 is extended;
3. A variant to evaluate the hydraulic role of the SBA concept if the SFR extension facility were to be located at the same depth as the present SFR (but unnecessary if a deeper depth is chosen, as turns out to be the case);
4. A large number of realizations of the DFN and PDZs (possible deformation zones) to address stochastic uncertainties.

Of these recommended variants, (1) is addressed directly in the temperate-case modelling for SR-PSU, by a range of variants detailed in SKB P-14-04 Section 4.2.3. Variant (2) does not seem to have been propagated to SR-PSU according to the same report. Variant (3) is made moot by the final choice of facility depth. The fourth item (not really a variant but a recommendation) has been addressed by carrying out flow simulations for a large number of stochastic realizations, although only three realizations are propagated in the safety assessment, as high-, low-, and intermediate-flow HRD cases.

With the exception of (3) this can be viewed as a reasonable approach to address the uncertainties that SKB has identified. An explanation should be sought as to why SKB apparently did not deal with the question of uncertain extent of ZFM871.

According to SKB P-14-04 (Öhman et al., 2014), the local parameterisation of deformation zones that intersect disposal rooms (primarily ZFMNNW1209 and ZFMWNW0835) is identified as a key uncertainty for the evaluation of cross flows through the disposal rooms. Alternative parameterizations of the HCDs are considered, including heterogeneous HCDs. A concise summary of the cases considered is given in Tables 2-1, 2-2, and 4-4 of P-14-04.

A more detailed review is recommended of the variants for depth dependence and heterogeneity of properties in the steeply dipping HCDs (along with the gently dipping HCDs) to ensure that the key uncertainties are adequately addressed, but at the level of consideration for this initial-stage review, the scope seems likely to be adequate.

More detailed review is also recommended of the specific HRD realizations that were chosen for propagation to radionuclide transport models, and whether these three high/low/intermediate-flow realizations are sufficient to bound the key uncertainties. For example, could a different high-flow realization yield a significantly different direction for near-field flows, and/or significantly different relative magnitudes of flow to different waste disposal vaults that could lead to different results in the dose and risk calculations?

2.3.2. Parameterization of regolith layers

Parameterisation uncertainty for the offshore marine sediments which control flow between sea and bedrock does not seem to have been evaluated for future climate conditions in the surface/shallow groundwater flow modelling (Werner et al., 2013). The hydrogeological modelling (Odén et al. 2014, Section 4.3.1) only considers a single set of regolith properties, although attention is given to the influence of the SFR pier.

SKB’s modellers have used the uncertain hydraulic properties of marine sediments, including a hypothetical “choke effect” attributed to convergence of flow through these sediments into bedrock fractures (Öhman et al., 2012, Section 4.7.1), as calibration factors to improve the ability of the hydrogeological models to measured inflows to the existing SFR. Hence the hydraulic properties of marine sediments appear to be significant for site understanding as well as quantitative predictions of flow to the proposed extended SFR facility, and therefore are recommended as a topic for more detailed review.

2.3.3. Characteristics of gently-dipping structures

Uncertainties in the occurrence and size, nature and transmissivity of gently dipping small-scale structures (minor deformation zones and discrete fractures) in shallow bedrock, and possible compartmentalization of flow due to heterogeneity or channelling, are not directly addressed in the hydrogeological modelling for SR-PSU as described by Odén et al. (2014).

The eight structures comprising the Shallow Bedrock Aquifer (SBA) are simply taken from the earlier hydrogeological modelling for SDM-PSU (Öhman et al., 2011), according to a very brief statement on p. 38 of Odén et al. (2014). More detailed review of the SDM-PSU modelling work (discussed in a separate review) could yield an appraisal of the significance of this uncertainty.

2.3.4. Limitations of borehole measurement programme

The SDM-PSU report (TR-11-04, p. 236) recommended sensitivity studies if no additional boreholes were drilled to investigate the potential for more high transmissivities outside of the deterministic deformation zones. The boreholes listed as the source of primary data from drilling campaigns Section 2.1 of Odén et al. (2014) are all represented in the more detailed account of data used in SDM-PSU (Öhman et al., 2011, Table 1-3), so it appears that no additional boreholes were drilled to address this recognized uncertainty in SDM-PSU.

Related uncertainties in the Hydro-DFN model, as mentioned in SDM-PSU, include uncertainty due to the practical detection limit of the PFL-f method, decreasing borehole sample size with depth (affecting estimates of trends in transmissivity with depth), limited sample size for parameterization of the Shallow and Deep domains of HRD, and conceptual questions about the reasons for systematically lower transmissivity inside the central block compared with closer to the Southern and Northern Boundary belts.

These uncertainties could motivate analysis of, e.g.:

- Parametric variants of the stochastic models based on sensitivity to the PFL-f detection limit and limited sample size at depth;
- Alternative models of DFN heterogeneity including non-stationary stochastic models to reflect differences between different subdomains;
- Alternative models or parameterizations for the Shallow and Deep domains.

However the HRD realizations mentioned by Odén et al. (2014, Table 4-2) and the supporting P-series report for the temperate case (Öhman et al., 2014, Section 4.2.1) are apparently all based on a single stochastic model of the DFN and PDZs. Thus neither parametric variants of the stochastic models nor alternative conceptual models for DFN heterogeneity have been analysed as part of SR-PSU.

2.3.5. Tunnel inflow measurements and decreases over time

In the SDM-PSU report, uncertainty was noted in measurements of inflow data due to removal of water as vapour via the ventilation system. It is surprising that measurements are not available for quantitative assessment of this effect and its seasonal variation, as the effect has been recognized at least since the Stripa Project when methods for measuring this component of the water budget based on psychrometry and airflow measurements of ventilation air were described and applied (Wilson et al., 1983).

According to Öhman et al. (2012, SKB-R-11-03 p. 48) based on personal communications with no specified date there were no measurements of the humidity of the air going through the ventilation of the SFR facility. Öhman et al. (2012) gave scoping estimates based on general meteorological data which indicate that the ventilation air could account for roughly 30 L/min condensation inflow during summer, or 30 L/min evaporative outflow during winter. This estimated seasonal fluctuation of 60 L/min amounts to 13% of the total inflow measured from pumping stations (Öhman et al., 2012, Table 4-1).

If SKB still has not been making at least periodic measurements of ventilation air humidity even after Öhman et al. (2012) raised the issue, this is a deficiency in the hydrologic monitoring programme for SFR that should be remedied. A request for complementary information on this topic could be useful to check if data have been gathered since 2012, and if not to ensure that such data will be gathered in the future on a regular basis.

The observations of decreasing inflow in the SFR tunnels over time could be explained by various hypotheses as listed by Öhman et al. (2012, p. 47). Most – but possibly not all – of these hypotheses are reversible in the post-closure period. For example fracture sealing by chemical precipitation is not necessarily reversible.

The lack of a clear conceptual understanding of the reason for declining inflows, combined with the lack of data to assess inflow and outflow of water via the ventilation air, implies corresponding uncertainties in the parameterizations of hydrogeological models that have been calibrated to inflows, and also estimates of resaturation times. These uncertainties should at least be discussed with an eye toward how the uncertainties propagate to the understanding of system evolution and radionuclide transport.

3. Suggestions for further review

3.1. Potential review topics related to key scenarios

Considering the scenarios that have been assessed in SR-PSU, the following scenarios related to hydrogeological factors considered in this review stand out as the ones that produce doses in excess of the dose corresponding to the risk criterion, or doses close to that level:

1. Intrusion wells;
2. High flow in bedrock combined with either rapid degradation of concrete barriers and waste containers, or high concentrations of complexing agents;
3. High flows in the repository;
4. Wells downstream of the repository;
5. Earthquakes.

The intrusion-wells scenario is judged to be adequately handled in terms of hydrological issues, although the use of risk dilution methods based on present-day well densities in the Forsmark area could be questioned as a higher-level methodological review issue. Potential review topics for the remaining topics are suggested and discussed in the following subsections.

3.1.1. High flow in bedrock and/or in the repository

SKB's method for constructing the *high flow in bedrock* scenario, could be a topic for further review, taking into account an independent assessment of the uncertainties and simplifications of the hydrogeological site-descriptive model. The key question is whether SKB is justified in their argument that the probability of such elevated flows in all vaults is "considerably less than 10%" (Main report, p. 233), or if these high flows are simply realistic.

Detailed review is also recommended of the selection of specific HRD realizations that were chosen for propagation to radionuclide transport models. The key question is whether these three high/low/intermediate-flow realizations are sufficient to bound the uncertainties that affect the dose and risk calculations. For example, could a different high-flow realization yield a significantly different direction for near-field flows, and/or significantly different relative magnitudes of flow to different waste disposal vaults that could lead to different results in the safety assessment?

Concerning the stochastic models for the DFN and PDZs that underpin the HRD realizations, neither parametric variants nor alternative conceptual models have been analysed as part of SR-PSU. The detailed review should identify whether any plausible parametric variants or alternative models are likely to give results that would lead to higher doses.

A more detailed review is also recommended of the variants for depth dependence and heterogeneity of properties in the steeply dipping HCDs (along with the gently dipping HCDs) to ensure that the key uncertainties are adequately addressed.

3.1.2. Degradation of engineered barriers

Calculations of repository-scale flows for the different concrete degradation states, for three different shoreline positions, are described in Section 6.2.1 of Abarca et al. (2013), but it is not fully clear how these calculations were utilised in the radionuclide transport and dose calculations. This could perhaps be resolved by a request for complementary information.

A broader topic for review is whether the hydraulic properties of concrete barriers and waste packaging, as used in the calculations of near-field flow rates, are adequately realistic, in terms of heterogeneity and how it evolves due to various degradation processes including development of fracturing. The hydraulic consequences of fracturing processes of concrete components are barely discussed in the process reports, and this review did not find any explicit analysis of the impacts on flows, apart from the stylized treatment of degradation states represented by the main scenario and the accelerated degradation scenario. Models for near-field flow by Abarca et al. (2013) have apparently assumed that the concrete has homogeneous properties at every stage.

An interdisciplinary review of SKB's handling of concrete degradation processes and their impacts on flow processes is therefore recommended, involving experts in concrete barriers, hydrogeology, and hydrogeochemistry. Specific topics could include the effects of (1) carbonatisation during the operational phase, (2) leaching of calcium carbonate by groundwater seeping through the matrix, and (3) development of fracturing, in terms of consequences for bulk hydraulic properties as well as heterogeneity within the concrete. The findings could inform an evaluation of whether SKB's analysis has considered an adequate range of concrete barrier properties, for the purposes of the safety assessment.

3.1.3. Wells downstream of the repository

The *wells downstream of the repository* scenario merits further review to assess the conservatism of the analysis by Werner et al. (2013), and consider the potential impact of uncertainty in the shallow bedrock hydrogeological model. The sensitivity of the risk scaling method also merits examination, to consider the influence of uncertainty in hydrogeological parameters, the density of wells in the area, and assumptions about future uses of wells on the risk calculation. As a higher-level methodological issue, the appropriateness of the safety function *avoid wells in the direct vicinity of the repository* should be critically examined, as there is no clear way to avoid future wells as a matter of repository design or construction features.

3.1.4. Earthquakes

The effects of earthquakes have been assessed based on calculations for a scenario in which the engineered barriers of the silo are breached. As part of SSM's review of the earthquake scenario, it is suggested that SSM's seismic and rock mechanics experts evaluate whether an earthquake scenario leads to a likelihood of any other significant changes in hydraulic properties, either in terms of breaching of the engineered barriers for other vaults, or by shear dilation of fractures in the near-field bedrock.

3.2. Other topics

3.2.1. Resaturation processes and duration

SKB has not modelled the resaturation period, arguing that the expected short duration of this period makes it reasonable to neglect details of the saturation process. This argument in turn relies on a 2001 modelling study (Holmén and Stigsson, 2001) which indicated rapid resaturation, on a time scale of 25 years. This modelling study used a continuum representation of the bedrock, and was based on an early version of the site-descriptive model that included only a few of the large transmissive structures that are described in SDM-PSU. Calibration was based on inflow measurements which are acknowledged to have significant uncertainties in the current site description, and required adjustment of various “skin factors” to constrain flows into the tunnels.

The robustness of the resaturation period estimates assumed in SR-PSU should be re-examined, considering the latest version of the site descriptive model and alternative assumptions regarding the reasons for apparent “skin effects” in tunnels along with uncertainties in tunnel inflow measurements.

3.2.2. Shallow groundwater system

Parameterisation uncertainty for the offshore marine sediments which control flow between sea and bedrock was identified as a key uncertainty in SDM-PSU, but does not seem to have been evaluated for future climate conditions in the surface/shallow groundwater flow modelling (Werner et al., 2013). The hydrogeological modelling (Odén et al. 2014) likewise only considers a single set of regolith properties, although attention is given to the influence of the SFR pier.

As noted in Section 2.3.2, SKB’s modellers have used the uncertain hydraulic properties of marine sediments, including a hypothetical “choke effect,” as calibration factors to improve the ability of the hydrogeological models to measured inflows to the existing SFR. Hence the hydraulic properties of marine sediments appear to be significant for site understanding as well as quantitative predictions of flow to the proposed extended SFR facility.

Seasonal fluctuations in groundwater levels are not modelled as part of SR-PSU (SKB TR-14-05, p. 60). Considering the shallow depth of the facility, it should be checked whether seasonal fluctuations in the water table could contribute significantly to dispersion in the far-field, or other aspects of transport.

Possible future human actions involving water management or underground construction that could affect the groundwater flow system at shallow depths have only been discussed qualitatively in SR-PSU. A more thorough review of possible human actions and their potential hydrological consequences is therefore motivated.

4. References

Emborg, M., Jonasson, J-E., and Knutsson, S., 2007. Långtidsstabilitet till följd av frysning och tining av betong och bentonit vid förvaring av låg och medelaktivt kärnavfall i SFR 1. SKB R-07-60, Swedish Nuclear Fuel & Waste Management Co.

Geier, J., 2015. Review of hydrogeological site-descriptive model SDM-PSU – Initial review phase. SSM draft report 15 Sep 2015.

Holmén, J.G., and Stigsson, M., 2001. Model of future hydrogeological conditions at SFR. SKB R-01-02, Swedish Nuclear Fuel & Waste Management Co.

Holmén, J.G., Stigsson, M., Marsic, N., and Gylling, B., 2003. Modelling of groundwater flow and flow paths for a large regional domain in northeast Uppland: A three-dimensional, mathematical modelling of groundwater flows and flow paths on a super-regional scale for different complexity levels of the flow domain, SKB R-03-24, Swedish Nuclear Fuel & Waste Management Co.

Painter, S., and Sun, A., 2005. Representation of an open repository in groundwater flow models. SKB R-05-10, Swedish Nuclear Fuel & Waste Management Co.

Pusch, R., 2003. Design, construction and performance of the clay-based isolation of the SFR silo. SKB R-03-30, Swedish Nuclear Fuel & Waste Management Co.

SKB 2010. Data report for the safety assessment SR-Site. SKB TR-10-52, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., 2010. DarcyTools version 3.4, Verification, validation and demonstration. SKB R-10-71, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., and Follin, S., 2010. Groundwater flow modelling of the excavation and operation phases – Forsmark. SKB R-09-19, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., and Ferry, M., 2010. DarcyTools version 3.4, User's Guide. SKB R-10-72, Swedish Nuclear Fuel & Waste Management Co.

Svensson, U., Ferry, M., and Kuylenstierna, H-O, 2010. DarcyTools version 3.4. Concepts, methods and equations. SKB R-07-38, Swedish Nuclear Fuel & Waste Management Co.

C.R. Wilson, C.R., Witherspoon, P.A., Long, J.C.S., Galbraith, R.M., DuBois, A.O., and McPherson, M.J. 1983. Large-scale hydraulic conductivity measurements in fractured granite. International Journal of Rock Mechanics and Mining Science & Geomechanics Abstracts 12/1983; 20(6):269-276. DOI:10.1016/0148-9062(83)90596-X.

Reports included in review assignment

Abarca et al., 2013. Flow modelling on the repository scale for the safety assessment SR-PSU. SKB TR-13-08

Odén et al., 2014. SR-PSU Bedrock hydrogeology. Groundwater flow modelling methodology, setup and results. SKB R-13-25.

SKB, 2011. Site description of the SFR area at Forsmark at completion of the site investigation phase. SDM-PSU Forsmark. SKB TR-11-04, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2013a. Climate and climate-related issues for the safety assessment SR-PSU. SKB TR-13-05, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2013b. Bedrock hydrogeology - Groundwater flow modelling. Site investigation SFR. SKB R-11-10, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014a. Safety analysis for SFR long-term safety main report for the safety assessment SR-PSU. SKB TR-14-01, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014b. Initial state report for the safety assessment SR-PSU. SKB TR-14-02, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014c. Waste form and packaging process report for the safety assessment SR-PSU. SKB TR-14-03, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014d. Engineered barrier process report for the safety assessment SR-PSU. SKB TR-14-04, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014e. Geosphere process report for the safety assessment SR-PSU. SKB TR-14-05, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014e. FEP report for the safety assessment SR-PSU. SKB TR-14-07, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014f. Radionuclide transport and dose calculations for the safety assessment SR-PSU. SKB TR-14-09, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014g. Model summary report for the safety assessment SR-PSU. SKB TR-14-11, Swedish Nuclear Fuel & Waste Management Co.

SKB, 2014h. Input data report for the safety assessment SR-PSU, SKB TR-14-12, Swedish Nuclear Fuel & Waste Management Co.

Vidstrand, P., Follin, S., and Öhman, J., 2014. SR-PSU Hydrogeological modelling. TD13 - Periglacial climate conditions. SKB P-14-06, Swedish Nuclear Fuel & Waste Management Co.

Werner et al., 2013. Hydrology and near-surface hydrogeology at Forsmark – synthesis for the SR-PSU project. SKB R-13-19, Swedish Nuclear Fuel & Waste Management Co.

Öhman, J., Bockgård, N., and Follin, S., 2012. Bedrock hydrogeology – Groundwater flow modelling. Site investigation SFR. SKB R-11-10, Swedish Nuclear Fuel & Waste Management Co.

Öhman, J., Follin, S., and Odén, M., 2013. SR-PSU Hydrogeological modelling. TD11 – Temperate climate conditions. SKB P-14-04, Swedish Nuclear Fuel & Waste Management Co.

Öhman, J., Follin, S., and Odén, M., 2014. SR-PSU Hydrogeological modelling. TD11 – Temperate climate conditions. SKB P-14-04, Swedish Nuclear Fuel & Waste Management Co.

Öhman, J., and Vidstrand, P., 2014. SR-PSU Bedrock hydrogeology. 0TD12 - Water-supply wells in rock. SKB P-14-05, Swedish Nuclear Fuel & Waste Management Co.

APPENDIX 1

Coverage of SKB reports

The following reports have been covered in the review (Table A1:1).

Table A1:1 Reports covered in review.

Reviewed report	Reviewed sections	Comments
SKB TR-13-08 Flow modelling on the repository scale for the safety assessment SR-PSU.	All	
SKB TR-14-01 Safety analysis for SFR long-term safety main report for the safety assessment SR-PSU.	All	Referred to mainly to provide safety-assessment context for hydrological sections.
SKB TR-14-02 Initial state report for the safety assessment SR-PSU	Sections on hydrogeological variables under 12.1.x – 12.8.x	
SKB TR-14-03 Waste form and packaging process report for the safety assessment SR-PSU	3.3 & 4.2 hydraulic processes	
SKB TR-14-04 Engineered barrier process report for the safety assessment SR-PSU	5.2, 6.2, 7.2, 8.2, 9.2 & 10.2	
SKB TR-14-05 Geosphere process report for the safety assessment SR-PSU	Section 3 hydraulic processes	
SKB R-13-19 Hydrology and near-surface hydrogeology at Forsmark – synthesis for the SR-PSU project.	All	
SKB R-13-25 SR-PSU Bedrock hydrogeology. Groundwater flow modelling methodology, setup and results	All	
SKB P-14-04 SR-PSU Hydrogeological modelling. TD11 – Temperate climate conditions.	All	Brief review; gives details of models presented in R-13-25.
SKB P-14-05 SR-PSU Bedrock hydrogeology. 0TD12 - Water-supply wells in rock	All	Brief review; gives details of models for well scenarios.
SKB P-14-06 SR-PSU Hydrogeological modelling. TD13 - Periglacial climate conditions	All	Brief review; gives details of models presented in R-13-25.
SKB TR-14-09 Radionuclide transport and dose calculations for the safety assessment	All	Focused on use of hydrogeological results

SR-PSU		in transport models.
SKB TR-14-12 Input data report for the safety assessment SR-PSU	Hydrology-related AMF items.	Used as reference to trace source of inputs to, and use of outputs from hydrogeological modelling.
SKB TR-13-05 Climate and climate-related issues for the safety assessment SR-PSU	Overview	Used as background for review.
SKB TR-14-07 FEP report for the safety assessment SR-PSU	Hydrology-related FEPs only.	Used as background for review.
SKB TR-14-11 Model summary report for the safety assessment SR-PSU	Sections on DarcyTools, COMSOL, Ecolego and MIKE-SHE models.	Used as background for review.
SKB TR-11-04 Site description of the SFR area at Forsmark at completion of the site investigation phase. SDM-PSU Forsmark	All	Focus of separate review of SDM-PSU; here used as background.
SKB R-11-03 Bedrock hydrogeology. Site investigation SFR	All	Focus of separate review of SDM-PSU; here used as background.
SKB R-11-10 Bedrock hydrogeology - Groundwater flow modelling. Site investigation SFR	All	Focus of separate review of SDM-PSU; here used as background.
SKB R-08-67 Geovetenskapligt undersökningsprogram för utbyggnad av SFR (in Swedish).	Sections related to hydrogeological investigations.	Part of separate review of SDM-PSU; here used as background

APPENDIX 2

Suggested needs for complementary information from SKB

1. As a supplement for more efficient use of the Assessment Model Flowchart (AMF) given in Appendix B of SKB TR-14-12, a sequential index to the numbered AMF data transfer items would be helpful, or better yet, an electronic version of the with hyperlinks to the explanatory text in SKB TR-14-12.
2. Access to datasets as given in SKB TR-14-12 will be needed for detailed review. Web links to the datasets are given but apparently require a security code to access. From a positive perspective, these links, once accessible, could obviate the need for numerous requests for complementary information that could be satisfied by access to detailed datasets
3. Data for particle tracks transferred from hydrogeological models to Ecolego (as described in Appendix A of TR-14-09, p. 226) would allow further analysis of dispersion and other pathway properties by SSM.
4. A more thorough discussion is needed of the hydrological consequences of fracture-generating processes in the waste containers and engineered barriers.
5. An explanation should be offered for the lack of periodic measurements of ventilation air humidity that could be used to estimate effects of ventilation air on SFR inflow measurements, and also any psychrometric data obtained since this issue was pointed out by Öhman et al. (2013).
6. A justification should be given for why SKB did not explicitly deal with the question of uncertain extent of ZFM871, as was recommended in the SDM-PSU report.

APPENDIX 3

Suggested review topics for SSM

1. Review of SKB's method of constructing the high flow in bedrock scenario, taking into account an independent assessment of the uncertainties and simplifications in the hydrogeological site-descriptive model. Assess whether SKB's is justified in their argument that the probability of such elevated flows in all vaults is low
2. Detailed review is recommended of the selection of specific HRD realizations that were chosen for propagation to radionuclide transport models. The key question is whether these three high/low/intermediate-flow realizations are sufficient to bound the uncertainties that affect the dose and risk calculations. The detailed review should also identify whether any plausible parametric variants or alternative models are likely to give results that would lead to higher doses.
3. A more detailed review is recommended of the variants for depth dependence and heterogeneity of properties in the steeply dipping HCDs (along with the gently dipping HCDs) to ensure that the key uncertainties are adequately addressed.
4. An interdisciplinary review of SKB's handling of concrete degradation processes and their impacts on flow processes is recommended, involving experts in concrete barriers, hydrogeology, and hydrogeochemistry, to assess SKB's analysis has considered an adequate range of concrete barrier properties.
5. The robustness of the resaturation period estimates assumed in SR-PSU should be re-examined, considering the latest version of the site descriptive model and alternative assumptions regarding the reasons for apparent "skin effects" in tunnels along with uncertainties in tunnel inflow measurements.
6. The *wells downstream of the repository* scenario merits further review to assess the conservatism of the analysis and to consider the potential impact of uncertainty in the shallow bedrock hydrogeological model. The sensitivity of the risk scaling method also merits examination, to consider the influence of uncertainty in hydrogeological parameters, the density of wells in the area, and assumptions about future uses of wells on the risk calculation.
7. As a higher-level methodological issue, the appropriateness of the safety function *avoid wells in the direct vicinity of the repository* should be critically examined, as there is no clear way to avoid future wells as a matter of repository design or construction features.
8. As part of SSM's review of the earthquake scenario, seismic and rock mechanics experts should evaluate should whether an earthquake scenario leads to a likelihood of any significant changes in hydraulic properties of the bedrock or engineered barriers of vaults other than the Silo (which has been considered), either in terms of breaching of the engineered barriers for other vaults, or by shear dilation of fractures in the near-field bedrock.
9. Parameterisation uncertainty for the offshore marine sediments which control flow between sea and bedrock was identified as a key uncertainty in

SDM-PSU, but the consequences apparently were not evaluated in hydrogeological modelling for SR-PSU. The hydraulic properties of marine sediments including hypothesized “hydraulic choke” (convergence) effects appear to be significant for site understanding as well as quantitative predictions of flow to the proposed extended SFR facility. The consequences of this uncertainty for the safety evaluation should be scoped, along with the consequences of seasonal fluctuations in the water table.

10. Possible future human actions involving water management or underground construction that could affect the groundwater flow system at shallow depths have only been discussed qualitatively in SR-PSU. A more thorough review of possible human actions and their potential hydrological consequences is therefore motivated.

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4

Review of chemical evolution in rock and engineered barrier systems in SFR according to the safety assessment SR-PSU

Activity number: 3030014-1012
Registration number: SSM2015-1037
Contact person at SSM: Georg Lindgren

Summary

This assignment concerns the chemical conditions in the SFR repository and its surroundings. Two important aspects covered in this assignment are the characterization of the present natural hydrochemical conditions at the site and the assessment of how the repository construction may affect these conditions. The engineered barrier systems, mainly the concrete component, and the various waste forms are expected to exert an appreciable influence on the chemical conditions within and around the repository. The chemical conditions are also expected to gradually change within the time scale addressed by the SR-PSU assessment, which depend both on internal transformations such as degradation of concrete and metal components, and on the external gradual evolution of the groundwater conditions due to land rise and climate changes.

This document provides a review of the chemical evolution in rock and engineered barrier systems as described in the SR-PSU documentation. The review has been conducted with regard to:

- Completeness.
- Scientific soundness and quality.
- Adequacy of relevant models, data and safety functions.
- Handling of uncertainties.
- Safety significance.
- Quality in terms of transparency and traceability of information.
- Feasibility of manufacturing, construction, testing, implementation and operation.

It is concluded from this initial review that review that for the most part, there is good assessment of the characteristics, influences and uncertainties for the evolution of the site and engineered barriers regarding potential salinity changes, pH, and Eh in SR-PSU documentation. Text presented below highlights where coverage may be less than satisfactory and finally, there are suggestions for review topics for the future more detailed assessment of SR-PSU planned by SSM.

The following topics/issues require additional information from, and consideration by, SKB:

- An understanding of how the rock-groundwater system has responded to environmental changes in the past is a key issue in forecasting future behavior. SKB should be encouraged to carry out sampling of matrix pore waters in its future activities at the SFR site.
- There is an incomplete presentation of principal component analysis (PCA) for groundwaters at the SFR site, with data only for Cl^-, $\delta^{18}O$, δ^2H and SO_4 being presented by SKB to determine mixing relationships. A full dataset would allow an evaluation of the role of water-rock reactions in the past and future evolution of groundwaters at the site. SKB should carry out a more detailed PCA study of SFR groundwaters, investigating more groundwater species than published thus far.
- SSM should ask for further clarification from SKB regarding the links between the oxidation of organic matter and the reduction of sulphate in groundwaters at SFR. This reaction could be a key control of redox in the far-field (thus influencing radionuclide solubility and sorption).
- SSM should ask SKB why the presence of saline groundwater at repository levels by up-coning from depth was not considered as an ‘unlikely scenario’ in the SR-PSU assessment.

- SKB should be asked to offer explanations as to why there are marked differences between the composition of clay minerals at the SFR and Forsmark sites, despite (apparently) similar histories of water-rock reaction.
- SSM should ask SKB to clarify its understanding of redox in groundwaters at SFR, especially the link between measured Eh values in groundwater and the presence of redox-sensitive minerals (Fe-oxides, clays) in rock fractures. SKB's current interpretation is at best vague, and at worst, highly uncertain.
- SSM should ask SKB to clarify its understanding of grout-groundwater interactions taking note of previous publications on this topic not referred to in SR-PSU documentation.
- SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with saline groundwaters, especially with regard to:
    - effects of the formation of Friedel's salt upon pH;
    - the impact of Mg^{2+} in groundwaters on pH; and
    - the selection of models for calculation of activity coefficients of aqueous species in its modelling of concrete degradation.
- SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with carbonate in groundwater, especially with regard to:
    - the potential armouring of concrete fracture surfaces by calcite and the consequent lowering of ambient pH in the near-field; and
    - Further use of natural analogues of carbonation reactions to increase confidence in the results of numerical modelling of concrete degradation.
- The potential interaction of Fe^{2+} from anaerobic corrosion of steel with cement and concrete is a 'new' topic, and as such, relevant research has not been reported by other waste management agencies. Nevertheless, this issue could potentially have a large impact upon concrete degradation processes and near-field pH so that SSM needs to ask SKB what it plans to do about the issue in its future R&D programme.
- SSM should ask SKB for clarification of the issue of how bentonite might have resaturated with cement pore fluids in the Silo.

The following topics/issues are suggested for inclusion in the detailed review stage of the review of SR-PSU by SSM:

- SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB. This study should attempt to link observations of groundwater chemistry and mineralogical evidence from drillcores to produce a more holistic view of water-rock reaction at the SFR site.
- A re-evaluation of the potential for up-coning of saline groundwater from depth should be carried out to confirm SKB's conclusions on this issue.
- The report by Vidstrand et al. (Vidstrand et al., 2006) on the exclusion of the effects of salt exclusion during periglacial conditions should be reviewed to assess the validity of SKB's conclusion that any occurrence of salt exclusion in the past would have been flushed from the rock-groundwater system.
- The effects of saline groundwater on concrete degradation should be modelled to assess rates of degradation and potential changes to pH.

Contents

1. Introduction

The Swedish Radiation Safety Authority (SSM) received an application for the expansion of SKB's final repository for low and intermediate level waste at Forsmark (SFR) on the 19 December 2014. SSM is tasked with the review of the application and will issue a statement to the government for its consideration in due course. An important part of the application is SKB's assessment of the long- term safety of the repository, which is documented in the safety analysis named SR-PSU.

SSM's review is divided into an initial review phase and a main review phase. The work presented here forms part of the initial review phase. This phase of the review has a number of general objectives:

- a broad understanding of the application should be achieved.
- It shall be assessed if SKB's documentation is understandable and complete with regard to the information that is needed to be able to make an assessment of the application.
- The key review topics for the main review phase shall be identified. These are topics that will have a significant impact on the assessment if the application fulfills relevant requirements.

This assignment concerns the chemical conditions in the SFR repository and its surroundings. The two important aspects covered here are:

- the characterization of the present natural hydrochemical conditions at the site and;
- an assessment of how repository construction may affect the above conditions.

The engineered barrier systems, mainly the concrete components, and the various waste forms are expected to exert an appreciable influence on the chemical conditions within and around the repository construction. The chemical conditions are also expected to gradually change within the time scale addressed by SR-PSU, which depend both on internal transformations such as degradation of concrete and metal components, and on the external gradual transformation of the groundwater conditions due to land rise and climate variations. The chemical conditions within and around the repository are important since they exert an influence on:

- the release of radionuclides from the different waste forms;
- retardation and transport of radionuclides within the repository vaults and the surrounding bedrock;
- interactions, alterations and degradation of waste and engineered components in the repository.

SKB has addressed these aspects within the main scenario of SR-PSU, but also within some of the less likely scenarios and some of the residual scenarios.

The following general points have been included:

- familiarisation with SKB's documentation, giving a brief account of the structure and most relevant parts as well as the safety relevance of the review.
- Suggestion of important review topics for the main review phase and a description of their importance in view of the safety assessment results.
- Where applicable, the adequacy of relevant models, data and safety functions have been assessed as well as the handling of uncertainties.
- Assessment of the need for complementary information or clarifications that are deemed necessary to effectively assess the license application in depth.
- Assessment and brief evaluation of the overall quality of SKB's documentation, including a brief assessment of the structure, transparency, traceability, scientific soundness, as well as maturity of SKB's technical solutions and of SKB's methodology.

More specifically, the following topics have been addressed:

- A review of SKB's characterization of the present groundwater conditions.
- A review and assessment of the change in salinity, pH and Eh conditions as a function of time due to the emplacement of waste and engineered barrier materials at the site.
- A review of how well characteristics, expected influences and uncertainties related to the above mentioned topics have been addressed by the main safety assessment report SKB TR-14-01.

2. Relevant Documentation for SR-PSU

A number of reports and papers have been read and evaluated for this review (summarised in the Appendix, Table A-1) and are briefly described below.

The report TR-14-01 (SKB, 2014d) is the main report for the safety assessment, describing the initial groundwater chemistry in Section 4.8 (page 122-128), the reference evolution in Section 6 for the first 1 ka after closure (Sections 6.3.6, 6.3.7, and 6.3.8 describe geochemical evolution, chemical evolution of the waste domain and evolution of the engineered barriers respectively), with a similar arrangement of descriptions for the temperate climate domain after 1 ka (Section 6.4), and periods of periglacial climate domain after 1 ka (Section 6.5). Scenarios are described in Section 7, with a 'less probable' scenario of relevance being 'accelerated concrete degradation' in Section 7.6.3 (calculational results for this scenario in Section 9.3.3). The Conclusions Section of TR-14-01 (page 364 and following) has the following relevant statements defining the functions and geochemical requirements of the natural and engineered barriers:

- "*the rock also provides a stable chemical environment, including anaerobic conditions which contribute to protecting reducing conditions at repository depth. Reducing conditions imply that iron corrodes only slowly and that the mobility of certain safety critical radionuclides (particularly radioisotopes of uranium) is low*". (page 370).
- *"For the Silo, the pH-buffering function of the concrete and the grout keeps gas production due to microbial activity and iron corrosion low. The choice of concrete as an engineering material also ensures good sorption properties"*. (page 371).
- "*For 1BMA and 2BMA vaults, the long-term evolution of the flow-limiting ability of the concrete structure is associated with a transformation of cement minerals, and the flow-limiting function is maintained for at least 20,000 years*". (page 371).
- "*For 1BTF and 2BTF vaults, the pH-buffering function of the concrete and the grout keeps gas production due to microbial activity and iron corrosion low. The choice of concrete as an engineering material provides good sorption*". (page 371).
- "*For the BRT vault, the function of the concrete is to limit the water flow in and around the RPVs and to maintain high pH conditions in order to limit corrosion of steel. Limited corrosion delays the release of the surface contamination on the inside of the RPVs, as well as the release of neutron activation products*". (page 372).
- "*Sorption of radionuclides has been shown to be the main mechanisms controlling retardation in the repository. Sorption occurs mainly on the cementitious materials in barriers and waste packages. The sorption depends on the amount of available concrete surfaces, but also on the chemical composition of the water in the repository. The importance of sorption is strongly related to the chemical characteristics of individual radionuclides, including their redox state*". (page 373).
- "*The pH in BMA is maintained at such a level that microbial degradation of C-14-containing waste is kept so low that release of C-14 as methane gas will not be a dominant transport pathway*". (page 377).

Geochemical aspects of the evolution of the Forsmark site is described in Chapter 5 of TR-14-05 (SKB, 2014c). The following key processes are described: advection and mixing of solutes; diffusion of solutes; speciation and sorption; rock-water interactions in the rock matrix; water-rock interactions in fractures; microbial processes; degradation of grout; colloidal processes; methane hydrate formation; salt exclusion; and earth currents. Each of the processes in this list is discussed in terms of: a general description; dependence between process and geosphere variables; boundary conditions; model and experimental studies; natural analogues; time perspective; handling in the safety assessment; handling of uncertainties; and adequacy of supporting references.

Chemical processes in waste and waste packaging are discussed in Sections 3.5 and 4.4 of TR-14-03 (SKB, 2014e). For the most part, these are fundamental descriptions of relevant processes as related to conditions in SFR and are thus analogous to FEP descriptions. These processes are: advection; diffusion; sorption/uptake; colloid formation and transport; dissolution, precipitation and recrystallization; degradation of organics; water uptake/swelling; microbial processes; metal corrosion; and gas formation and transport.

The equivalent report for the engineered barrier system is TR-14-04 (SKB, 2014a) and has a similar layout and text content as TR-14-03 described above.

The FEP report for SR-PSU is TR-14-07 (SKB, 2014b) and provides direct links to the processes defined above in the 'Waste and Waste Packaging' (TR-14-03) and 'Engineered Barriers' (TR-14-04) process reports described above.

Detailed modelling of the evolution of the degradation of concrete in the BMA vaults is described in the report by Höglund (R-13-40 - Höglund, 2013). This includes modelling of both physical and chemical processes and is in much greater detail than similar studies published previously by SKB (e.g. Gaucher et al., 2005; Cronstrand, 2007). This report by Höglund is the mainstay for the understanding of concrete degradation as presented in the main report (TR-14-01).

A more simplistic and conservative assessment of the degradation of concrete is presented in the report by Cronstrand (Cronstrand, 2014) which treats the near-field as a mixing tank and deals with advection and equilibrium reactions only to model pH evolution with time.

Other underlying reports and papers that have been consulted are:

- R-11-06 (Nilsson et al., 2011) which presents the most detailed hydrogeochemical description for SR-PSU.
- P-11-25 (Gimeno et al., 2011) which describes mixing and water-rock interaction modelling of groundwater data from SFR.
- R-08-102 (Sandström et al., 2008) which describes fracture mineral data for the Forsmark site.
- P-11-01 (Sandström and Tullborg, 2011) which presents the main dataset for the mineralogical compositions of fractures at SFR showing that clay minerals like mixed-layer illite-smectite and illite dominate at SFR in contrast to Forsmark where corrensite (mixed layer chlorite-smectite) dominates.
- TR-14-05 (SKB, 2014c) which is a description of natural processes affecting the chemical evolution of groundwater at the SFR site. The report has a more balanced assessment of the role of different processes than that presented in TR-11-04, R-11-06, and P-11-25.

3. Current groundwater conditions

Hydrochemical data for the SFR site are presented in chapter 8 of the site description report SKB (SKB, 2011) and in more detail in Nilsson et al. (Nilsson et al., 2011), with water-rock modelling described in Gimeno et al. (Gimeno et al., 2011) and details of fracture mineralogy in Sandström and Tullborg (Sandström and Tullborg, 2011) and Sandström et al. (Sandström et al., 2011). These studies describe four major groundwater types at SFR:

1. Local Baltic Seawater type;
2. Littorina type water with a glacial component;
3. Brackish-glacial water type, and
4. Mixed brackish water (transition type).

SKB believes that the distribution of the different groundwater types shows that the major deformation zones have served as important groundwater flow pathways over long periods of geological time while single discrete fractures in rock volumes between zones generally contain older and more isolated groundwater. Currently, the steeply dipping geological structures in particular have facilitated the drawdown of modern Baltic Seawater which has been observed since excavation and construction of the SFR commenced some twenty years ago.

Some key geochemical features described by SKB are:

- Most of the SFR groundwaters seem to be in equilibrium or slightly oversaturated with respect to calcite.
- The main source of sulphur in the SFR groundwaters is the intrusion of past (Littorina) and present (Baltic) seawaters, which have mixed with the earlier resident groundwaters. According to the available isotopic data ($\delta^{34}S$), sulphate-reducing microbial activity seems to have played a minor role in determining dissolved sulphate concentrations, except in some of the brackish-glacial type groundwaters with low sulphate content and high $\delta^{34}S$ values. Also, some of the groundwaters with large fractions of present-day Baltic Sea waters exhibit SO_4/Cl ratios that suggest the existence of active sulphate-reducing processes, although the effect is small. Like the Forsmark groundwaters, all the SFR groundwaters are undersaturated with respect to gypsum and celestite and in equilibrium with respect to barite, calcite and fluorite.
- The potentiometric Eh measurements in the SFR groundwaters provide both positive and negative values. Reducing conditions (Eh values between −140 and −190 mV) are in line with those measured in the Forsmark groundwaters and are apparently caused by the occurrence of an iron phase with an intermediate crystallinity and/or by ferrous clay minerals, both of which have been identified.
- The redox capacity provided by the fracture minerals in the hydraulically conductive fractures is mainly found in Fe (II) present in chlorite and clay minerals (e.g. corrensite, a mixed-layer smectite-chlorite mineral) and to some extent in the less abundant sulphides (mainly pyrite). It is unclear however, which mineral assemblage may control redox conditions at depth.
- PCA (Principle Component Analysis) using the M3 code could not resolve perfect mixing proportions of the end-member waters that have contributed to the chemical composition of the SFR groundwaters.

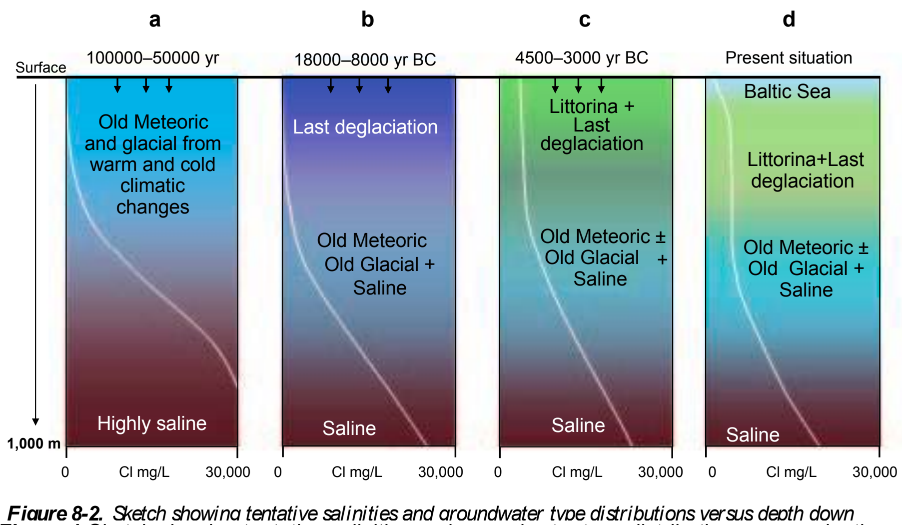

Figure 1 Sketch showing tentative salinities and groundwater type distributions versus depth down to 1000 m depth for the transmissive deformation zones at SFR (from SKB, 2011). From left to right: a) situation prior to the last deglaciation, b) last deglaciation and intrusion of Late Weichselian meltwater, c) Littorina Sea water penetration caused by density intrusion, and d) the present-day situation with possible penetration of local Baltic Sea water. The white line shows chloride concentration versus depth.

The hypothesized evolution of the hydrochemical system with time is illustrated in Figure 1.

With regard to groundwater interaction with the rocks, SKB (Sandström and Tullborg, 2011, Abstract; Nilsson et al., 2011, page 27) report that there are no *major* differences between the fracture mineralogy of the investigated borehole sections from SFR and the fracture mineralogy of the Forsmark site investigation area. The four fracture mineral generations distinguished within the Forsmark site investigation are also found at SFR. However, *some* differences have been observed:

- barite and uranium minerals are more common in the SFR fractures.
- Clay minerals like mixed layer illite-smectite and illite dominate at SFR in contrast to Forsmark where corrensite (mixed-layer chlorite-smectite) is the most common clay mineral.
- REE-carbonates which were not identified in the samples from the Forsmark site investigation occur on many of the analysed fracture surfaces at SFR.

Nilsson et al. (Nilsson et al., 2011, page 27) report that ‘Generation 4’ (i.e. most recent) fracture fillings consist predominantly of clay minerals and thin precipitates of calcite in hydraulically conductive fractures; minor occurrences of pyrite and goethite are also found. They believe that precipitation probably occurred at low temperatures (< 50 °C) during a prolonged period, possibly since the late Palaeozoic until present by groundwater circulation.

Some issues raised by the review of SKB documentation for hydrochemistry are:

- salinity;

- mixing and reaction;
- pH buffering;
- carbonate system, and
- redox reactions.

These topics are discussed in more detail below.

3.1. Salinity

The degree of salinity of the groundwater at the SFR site will control to a large extent the rate and amount of degradation of the concrete engineered barriers (degradation is enhanced under more saline conditions) and also the ambient pH of near-field pore fluids, thus impacting upon not only the timing of release of radionuclides from concrete vaults, but also their solubility and sorption behaviour (in general pH > 10 is desirable for safety-relevant time periods).

SKB (SKB, 2011; top of page 188) notes that the range in chloride concentration of the SFR groundwaters is small (1500 to 5500 mg/L Cl^-) compared with the Forsmark site investigation area (50 to 16,000 mg/L Cl^-). Moreover, SKB goes onto state that present-day groundwater chemistry at SFR is influenced by drawdown to the tunnel, which will be important in some of the sampled sections where inflow of Baltic Sea water can be expected. The most saline groundwater is generally found at intermediate depths (100-200 m) and is of the brackish marine Littorina type. The more dilute brackish water found at shallow depths (~100 m) is of local Baltic type, and the most dilute waters (1600 mg/L Cl^-) are of brackish-glacial type at about 240 m depth (SKB, 2011; foot of page 190).

Regarding changes to salinity during operation of SFR, SKB observes that most of the changes showed a slightly decreasing chloride concentration between 1986 and 2000 followed by a nearly stable period until 2010, with the greatest changes in groundwater pressure and inflow to the boreholes and the tunnel system occurring soon after construction (SKB, 2011; paragraph beneath bullet points on page 200).

Unlike Forsmark investigations, waters in the rock matrix (‘pore waters’) at SFR have not been sampled (SKB, 2011; section at foot of page 198) which makes it difficult to assess past natural variations of groundwater salinity. An understanding of how the rock-groundwater system has responded to environmental changes in the past is a key issue in forecasting future behaviour. *SKB should thus be encouraged to carry out sampling of matrix pore waters in its future activities at the SFR site.*

SKB has produced a schematic diagram of the distribution of water types at SFR, here reproduced as Figure 2. The precise location of deep saline water at SFR is hypothetical in Figure 2 since there are no data from boreholes deeper than -400 m elevation. However, a key issue for future behaviour of SFR must be the potential for up-coning of saline water from depth along the more transmissive southern and northern boundary belts. SKB refers to a ‘weak upward regional flow along these deformation belts (SKB, 2011; top of page 203). Moreover SKB (SKB, 2011; bottom of page 181) notes that most of the available data from SFR are concentrated around the disposal facility with the result that the hydrochemistry both laterally and vertically outside the facility is less well characterised, and the full extent of the drawdown/upconing mixing effects is still uncertain.

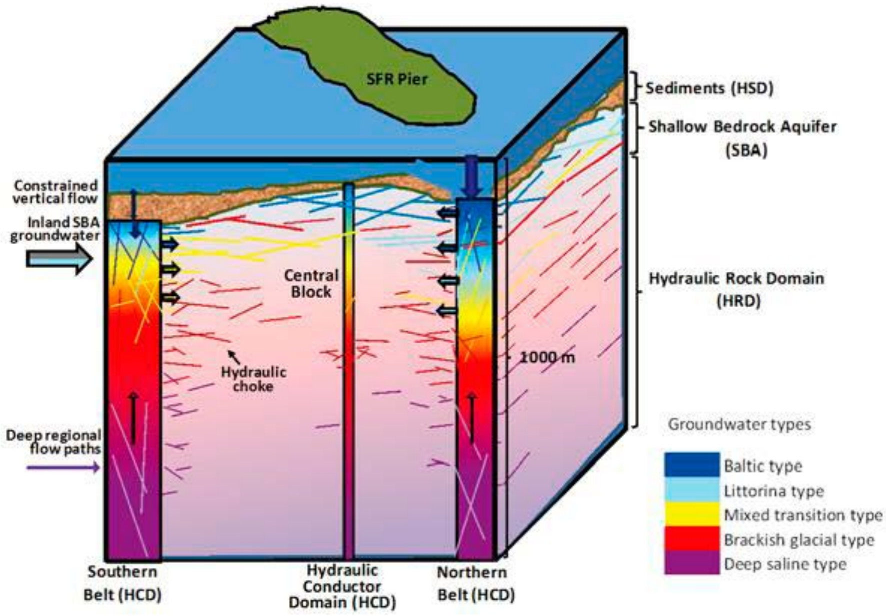

Figure 2 Conceptual block model (0–1000 m depth) integrating the major hydrogeological and hydrogeochemical features of the investigated SFR rock volume. The different groundwater types are indicated by the colour scheme displayed on the right hand side. The deep saline groundwater which is indicated by lilac is not present as a dominant groundwater type in the SFR rock volume. From SKB (SKB, 2011; page 203).

3.2. Mixing and reaction

The establishment of an understanding of the principal controls upon the chemical composition of groundwater during site characterisation activities enables a better understanding of how the rock-groundwater system may evolve during future perturbations caused by climate variations and/or engineered barrier degradation. For example, control of major element variations predominantly by groundwater mixing implies little or no buffering of important variables such as pH, Eh and PCO_2 due to reaction with the rock, especially with minerals lining fractures. pH, Eh and PCO_2 are instrumental in controlling the solubility and sorption behaviour of most radionuclides of interest for safety assessment.

SKB describes that groundwater samples reveal complex mixing patterns arising from the different evolutionary stages of the Baltic Sea, as well as from the presence of the SFR facility (SKB, 2011, top of page 182). SKB believes that the hydrochemical indicators Cl^-, Mg^{2+} and $\delta^{18}O$ show large variations linked to the origin and residence time of the groundwaters, despite the relatively small variation in salinity. Principal Component Analysis (PCA) using Cl^-, $\delta^{18}O$, $\delta^{2}H$ and SO_4 has been used to discriminate groundwater types based on these components. Nevertheless, modelling with the M3 mixing code could not resolve perfect mixing proportions of the end-member waters that have contributed to the chemical composition of the SFR groundwaters.

In its analysis, SKB emphasises mixing relationships to explain hydrochemical variations, and downplays reaction with the host rocks, despite good mineralogical information showing the presence of the solid products of water-rock reaction (carbonates, clays, zeolites) in hydraulically-active fractures (Sandström and Tullborg, 2011; Sandström et al., 2011). Nevertheless, SKB states (Nilsson et al., 2011, foot of first paragraph on page 47):

> "*the present groundwaters are a result of complex mixing and reactions over a long period of geological time. Mixing will be more important in those parts of the bedrock with dynamic hydrogeological properties, for example, the more conducting fractures and fracture zones in the SFR model volume. In other less dynamic parts, the groundwater chemistry will be more influenced by water/rock interaction processes and diffusion processes* ".

Consequently, there is a rather tenuous link made by SKB between the analysis of the hydrochemical data and the evidence from fracture fillings in the rock. This could be resolved by an analysis involving thermodynamic activity diagrams, such as that employed to interpret hydrochemical variations at Forsmark by SSM (e.g. Savage, 2011 - Figure 3). This omission is exemplified by SKB offering no explanation as to why clays lining fractures at SFR are dominated by illite and smectite-illite whereas those found during Forsmark site investigations are dominated by corrensite (mixed-layer smectite-chlorite) (Nilsson et al., 2011, text on page 27). It could be argued that very different water-rock reactions have operated at each site for which SKB has no current understanding, due principally to its focus upon groundwater mixing models to interpret hydrochemical data.

Despite the recognition (above) of the potential importance of water-rock reaction governing hydrochemical behavior, the five 'key water origins' defined by SKB (Nilsson et al., 2011, Section 3.2.2, page 47) omits definition of any origin (or modification) by water-rock reaction and instead lists 'saline water', 'brackish non-marine water', 'last de-glaciation meltwater', 'brackish marine (Littorina/Baltic) water', and 'fresh water' as key water types. Somewhat unusually, the concentrations of potassium and magnesium have been used by SKB as 'marine indicators' (Nilsson et al., 2011, last bullet point on page 48) in mixing calculations, despite the fact that both these elements are known to be reactive in seawater-rock systems (e.g. Sayles, 1979; Gieskes and Lawrence, 1981; Kastner et al., 1990; Savage et al., 1993; Moore et al., 2001), with both elements being susceptible to being removed through the formation of clays such as illite. SKB recognizes the reactive behavior of Mg (Nilsson et al., 2011, 2nd paragraph, page 50):

> "*almost all of the SFR and Forsmark samples are somewhat depleted in magnesium compared to the initial marine ratios indicated by the line representing the marine Mg/Cl ratio, due primarily to ion exchange reactions lowering the Mg value in the groundwater* ".

However, SKB does not define a reactive end-member in mixing calculations.

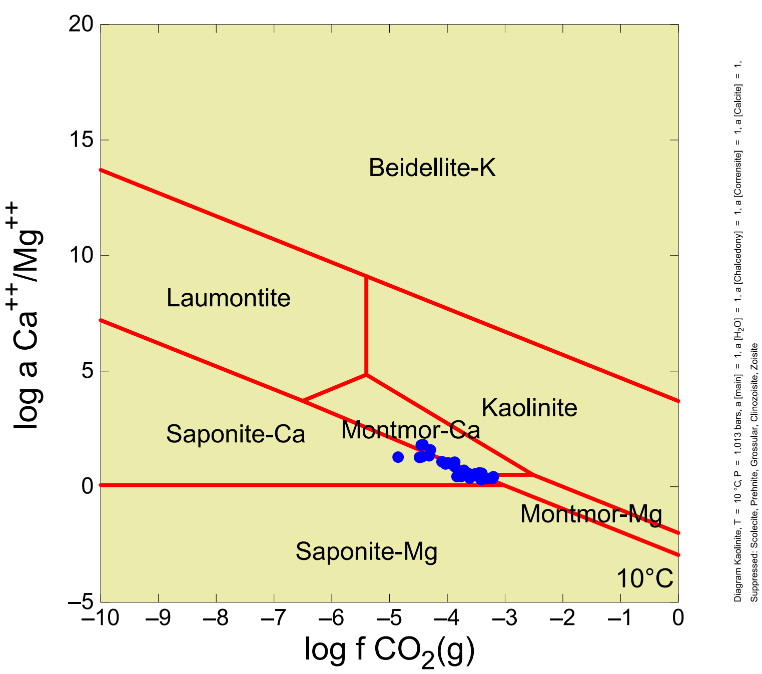

Figure 3 Mineral stabilities in the system CaO-MgO-K_2O-Al_2O_3-SiO_2-H_2O-CO_2 at 10 °C. Blue dots represent compositions of groundwaters from repository depth at Forsmark (data from A. Bath). Data suggest control of Ca/Mg, PCO_2 (and pH), by montmorillonite-saponite coexistence.

Another issue here relates to the scope of PCA calculations used by SKB to define mixing relationships. One of the advantages of the use of PCA is that it can reduce a large number of analytical variables into a few meaningful 'components' of variation. However, in its PCA analysis (Nilsson et al., 2011, Section 3.3.2, page 52), SKB chooses to reduce the number of input variables to four, namely Cl^-, SO_4^{2-}, δ^2H and $\delta^{18}O$. It is considered here that although this 'reduced' analysis may be useful in defining broad groundwater end-members, it is less rewarding in terms of the identification of potential rock-water reactions that may be important for the future evolution of the site.

In conclusion, it is suggested that this issue is pursued further by:

- requesting SKB to carry out a more detailed PCA study of SFR groundwaters, investigating more groundwater species than published thus far, and
- SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB.

3.3. pH buffering

The solubility and sorption of many radionuclides is sensitive to pH due to its role in affecting aqueous speciation.

Calcite is seen to be a major control upon pH in groundwaters at the SFR site (e.g. Gimeno et al., 2011, Section 4.1, page 39):

> "*Calcite is one of the most abundant minerals in fracture fillings in these sites and it plays an integral role in the pH-buffering of the recharge groundwaters. CO_2 partial pressure (usually referred as pCO_2 in this document) is another relevant parameter for understanding the evolution of the carbonate system and for evaluating possible uncertainties in measured pH values*".

However, there does not seem to be a clear understanding of pH-buffering reactions, or the carbonate system in general. Text at the start of the penultimate paragraph of page 43 of Gimeno et al. (Gimeno et al., 2011) states:

> "*Due to the fast dissolution kinetics of calcite compared with silicates and aluminosilicates, the presence of this mineral in significant amounts is important as it provides buffering capacity against acidification*".

This statement implies that calcite somehow acts alone in the pH buffering process, yet in the paragraph preceding the text above, states:

> "*The available mineralogical information for the fracture fillings present in the SFR bedrock, indicates that, together with chlorite, calcite is one the most abundant fracture filling minerals and is widely distributed at all examined depths (reaching 520 m.a.s.l.) without significant variations with depth (Sandström and Tullborg 2011). Clay minerals, mainly mixed layer smectite-illite and illite, also appear in dominant amounts in open fractures*".

Calcite is not an essential mineral of the rocks constituting the repository host rock at SFR, but is a product of water-rock reaction over geological time by reactions such as the irreversible weathering of the calcic component of plagioclase feldspar (anorthite, $CaAl_2Si_2O_8$) to form clays (here represented by illite, as observed in fracture-fillings at Forsmark):

$$3 \text{ anorthite} + 2 K^+ + 3 HCO_3^- + H^+ \rightarrow 2 \text{ illite} + 3 \text{ calcite}$$

Savage et al. (Savage et al., 1999a; Savage et al., 1999b) showed that the pH buffer capacity of solid carbonates is much less than that of aluminosilicate minerals in water-rock systems. Moreover, calcite is such an infinitesimal part of the mineralogical system at SFR that from mass balance constraints alone it is highly unlikely to constitute a significant pH buffer. Gimeno et al. (Gimeno et al., 2011, penultimate paragraph on page 43) envisage an ion exchange relationship between carbonates and clays, rather than one involving dissolution and precipitation:

> "*the important presence of clay minerals in the open, water conducting fractures would support the probable existence of cation exchange processes during the groundwater evolution and their participation in the control of calcium and other cations (calcium and potassium appear in significant amounts in the usually poorly ordered, mixed layer clays of smectite-illite type)* ".

This appears to be a basic misunderstanding of typical silicate weathering reactions which enable pH-buffering in rock-groundwater systems. It is also important to consider the rates of the respective reactions; silicates react much more slowly than carbonates, but may be more important buffers of pH in the longer term (for example, see Savage and Arthur, 1997).

Despite an origin by mixing being ascribed to most chemical species in SFR groundwaters, somewhat contradictorily, the origin of silica is ascribed to water-rock reaction (Gimeno et al., 2011, bottom of page 55):

> "*In groundwaters with short residence times, the main processes that can participate in the control of silica contents are incongruent dissolution of feldspars with formation of secondary clays, clay mineral transformations and silica adsorption-desorption reactions in clays (Langmuir 1997 and references therein). For the SFR, this type of situation can be inferred for recent Baltic waters circulating in some fractures (with or without minor mixing), for which silica contents are probably controlled by surface reactions in clays* ".

Nilsson et al. (Nilsson et al., 2011; foot of page 104) note that barite is common in SFR drillcores and that harmotome (Ba-zeolite) is also found. However, no explanation is offered for the origin of barium in SFR groundwaters. In crystalline rocks such as granites, barium is concentrated in K-feldspar. Dissolution of K-feldspar in the presence of sulphate dissolved in the groundwater will often lead to the precipitation of barite. The common occurrence of Ba-rich minerals is thus an indication of the participation of K-feldspar in water-rock reactions.

It is concluded therefore that water-rock reaction is invoked selectively by SKB to explain certain hydrochemical phenomena (pH, redox), but not others (controls of major element variations). This is inconsistent and the understanding of pH-controlling weathering reactions seems limited. Also, there is no current understanding for the differences in clay mineral compositions (important in pH and redox-controlling reactions) between the Forsmark and SFR sites.

This issue could be pursued further by:

- SSM carrying out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB (as suggested above). This study should attempt to link observations of groundwater chemistry and mineralogical evidence from drillcores to produce a more holistic view of water-rock reaction at the SFR site.

3.4. Carbonate system

The carbonate system is important for radionuclide migration in that the solubility and sorption of most actinides are sensitive to the amounts of bicarbonate ion in groundwater. It is thus important to understand controls (reactions) of PCO_2 in groundwater.

Groundwaters at SFR are shown to have PCO_2 values greater than that required for equilibrium with the atmosphere (log PCO_2 = -3.5 bars) (Gimeno et al., 2011, Section 4.1.3) and range up to log PCO_2 = -2.0 bars. Most groundwaters in fractured hard rocks have log $PCO_2 \leq$ -5.0 bars at 25 °C (e.g. Coudrain-Ribstein et al., 1998; Savage et al., 1999a), so it is difficult to envisage such high PCO_2 values in groundwaters at SFR without some form of organic carbon degradation through reactions such as:

$$2CH_2O(s) + SO_4^{2-} \rightarrow 2HCO_3^- + HS^- + H^+$$

Although this type of reaction is not discussed by Gimeno et al. (Gimeno et al., 2011), Nilsson et al. (Nilsson et al., 2011; bottom of page 98) state:

> "*high and variable HCO_3^- values are the result of the biological activity during infiltration of marine waters through the seabed sediments*".

Nilsson et al. (Nilsson et al., 2011; Conclusion section on page 105) also recognise that sulphate in SFR groundwaters is reduced microbially to sulphide (Nilsson et al., 2011; 3rd paragraph on page 103) but there is no direct link made by this author with the organic degradation reaction defined above. In the diagenesis of marine sediments, it is well-known that the generation of high PCO_2 in pore waters is a consequence of the (microbial) oxidation of organic carbon by sulphate to produce bicarbonate and sulphide ions (e.g. Andrews et al., 1996). Consequently, it is not clear why SKB has not linked sulphate reduction with high PCO_2 values in groundwaters at SFR which adds to the overall impression of relatively poor understanding of water-rock interaction processes.

Despite the importance of water-rock reaction for the carbonate system (and by implication, the behaviour of Ca in groundwaters), Nilsson et al. (Nilsson et al., 2011, page 101) go onto state:

> "*Although heterogeneous reactions (calcite re-equilibrium, cation exchange) may have noticeably modified the dissolved calcium concentrations, mixing control is still evident* ".

This issue should be resolved by SSM asking for further clarification from SKB regarding the links between the oxidation of organic matter and the reduction of sulphate in groundwaters at SFR. This reaction could be a key control of redox in the far-field (thus influencing radionuclide solubility and sorption).

3.5. Redox reactions

The solubility and sorption behaviour of many radionuclides (especially actinides) is sensitive to redox activity, with lower Eh tending to lower element solubility. Understanding the controls of redox in the far-field is thus key to the modelling of the migration and retardation of many radionuclides.

SKB's assessment of redox conditions at SFR are somewhat uncertain, with measured reducing Eh values ranging between -140 and -190 mV and oxidising values between +30 and +110 mV (SKB, 2011; foot of page 182). The reducing conditions are ascribed to either 'an iron phase' (*sic*) of indeterminate crystallinity, or by 'ferrous clay minerals'. 'Redox capacity' is ascribed to the presence of chlorite and Fe-bearing clay minerals in fracture fillings.

Interestingly, although SKB consider that major variations in hydrochemical conditions can be attributed mainly to mixing of groundwater types, heterogeneous reactions between minerals and groundwater are relied upon to provide stable redox conditions. This assessment by SKB seems somewhat inconsistent, since the equilibration (dissolution-precipitation) of sheet silicates such as biotite (the dissolution of which is seen as the source of fluoride in SFR groundwaters – foot of page 106 of Nilsson et al., 2011), chlorite and clay minerals will contribute solutes other than reduced iron to groundwaters.

SSM should ask SKB to clarify its understanding of redox in groundwaters at SFR, especially the link between measured Eh values in groundwater and the presence of redox-sensitive minerals (Fe-oxides, clays) in rock fractures. SKB's current interpretation is at best vague, and at worst, highly uncertain.

4. Evolution of pore water conditions

4.1. Site evolution

This aspect is principally discussed in Section 5 of the Geosphere Process Report (SKB, 2014c). In this report, a number of processes are highlighted that could impact upon pore fluid chemistry in the rock and near-field, namely:

- advective transport/mixing of dissolved species;
- reactions between groundwater and rock matrix;
- dissolution-precipitation of fracture-filling materials;
- degradation of grout;
- salt exclusion.

Some comments on SKB's analysis are provided on these topics below.

4.1.1. Advective transport/mixing of dissolved species

SKB recognises that advective transport and mixing can have a direct impact upon groundwater composition (SKB, 2014c; top of page 109). It is not clear however, how such processes accommodate water-rock reaction in SKB's modelling work (see below).

It is noteworthy that SKB rules out any upward mixing of more saline groundwaters from depth during the initial temperate period (SKB, 2014c; page 103, 5th paragraph):

> "*Further, high-saline groundwater from deeper parts (SKB 2013b) will not influence the groundwater. Thus, low salinity groundwater will prevail during this initial period of temperate climate domain* ".

It is not clear why SKB has ruled out this uncertainty and this issue should be pursued further by SSM since the presence of saline groundwaters would accelerate the degradation of concrete barriers due to enhanced solubilities of cement solids at higher salinity. This would require an analysis from a physical hydrogeological perspective.

4.1.2. Reactions groundwater/rock matrix

This section in SKB's geosphere process report (SKB, 2014c; Section 5.5) envisages a greater role for water-rock reaction in the overall moderation of groundwater compositions than seen elsewhere in the SFR-PSU assessment such as for pH (SKB, 2014c; page 138, 5th paragraph):

> "*The rock's minerals are of importance for the groundwater pH. There is a direct influence that is dependent on the interaction between the water and readily soluble minerals such as calcite, and an indirect influence that is*

> *controlled by slow weathering, the chemistry of the water and microbial conditions* ".

This statement is inconsistent with views and analysis expressed elsewhere by SKB where the role of groundwater mixing rather than water-rock reaction is stressed (e.g. Nilsson et al., 2011; Gimeno et al., 2011). This type of inconsistency (presumably between different contractors for SKB) has been noted before by SSM in the review of documentation for the licence application for the construction of the spent fuel repository at Forsmark (e.g. Savage, 2012). Such inconsistencies lead to an impression that the past evolution of the geochemical system at the SFR site is not sufficiently well understood to be able to predict how the rock-groundwater system will behave when perturbed by future natural (climate changes) and engineered (repository construction and degradation) perturbations.

SKB's position regarding Eh is similar ((SKB, 2014c; page 138, 6th paragraph):

> "*The bedrock content of reducing substances such as sulphide, divalent iron and manganese is vital for maintaining reducing conditions in the groundwater. The reducing capacity available in the rock matrix at SFR exists mainly in the Fe(II)-bearing biotite, chlorite, amphibole, pyrite and magnetite. Biotite is, by far, the main reducing mineral in the rock matrix at SFR (Sandström and Stephens 2009, Curtis et al. 2011, Sidborn et al. 2010)*".

Although the role of water-rock reaction is thus acknowledged regarding the control of redox, the contributions that dissolution of biotite, chlorite, amphibole, pyrite and magnetite would make to the control of groundwater composition with respect to major elements such as potassium, magnesium, iron and silicon is somehow unrecognised. Again, this suggests a somewhat confused interpretation of groundwater chemical evolution that does not instil confidence in SKB's predictions of future behaviour.

Nevertheless, Section 5.5 concludes that:

> "*Rock minerals are taken into account in the assessment of evolution of groundwater composition (Román-Ross et al. 2014[1])".*

This statement is thus rather contradictory with the assessment made here and in conclusion, it is considered that SKB needs to make more use of mineralogical and thermodynamic data in its assessment of hydrochemical evolution.

To re-iterate statements from previous sections of this report on these topics:

- SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB. This study should attempt to link observations of groundwater chemistry and mineralogical evidence from drillcores to produce a more holistic view of water-rock reaction at the SFR site.
- SSM should ask SKB to clarify its understanding of redox in groundwaters at SFR, especially the link between measured Eh values in groundwater and

[1] A copy of this report could not be found on SKB's website.

the presence of redox-sensitive minerals (Fe-oxides, clays) in rock fractures. SKB's current interpretation is at best vague, and at worst, highly uncertain.

4.1.3. Dissolution-precipitation of fracture-filling materials

The Geosphere Process Report states that (SKB, 2014c; 1st sentence of Section 5.6.1 on page 145)

> "*Minerals on fracture surfaces can dissolve in the groundwater and, conversely, solutes in the groundwater can precipitate on fracture surfaces. These processes are in general controlled by the advection of solutes and mixing of groundwaters".*

However, emphasis is placed upon the latter process (advection/mixing) in the description of groundwater evolution presented elsewhere in SR-PSU. Although the Geosphere Process Report also states that (SKB, 2014c; page 146, 1st sentence of paragraph 3):

> "*Precipitated fracture minerals, such as calcite, pyrite, zeolites and iron oxides, make it possible to draw conclusions concerning the water chemistry that prevailed when the minerals were formed ".*

In general, little use of these mineralogical observations is made in the main SR-PSU reports.

There are many references to the apparent stability of calcite in fractures in the bedrock at SFR (e.g. SKB, 2014c; page 147, 4th paragraph):

> "*no evidences for calcite dissolution in the upper parts of the bedrock have been found* ".

However evidence from SEM investigations carried out by Sandström et al. (Sandström et al., 2011) clearly show features of calcite that are attributable to dissolution (Figure 4) which challenges the statement above that calcite is stable in the ambient rock-groundwater system. It could be concluded therefore that SKB's hydrochemical interpretation of the SFR site is incorrect such that the immersion of the rock-water system with brackish groundwater (of old Littorina and Baltic seawater origins) is leading to a progressive decrease in ambient pH and dissolution of calcite.

SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB. This study should attempt to link observations of groundwater chemistry and mineralogical evidence (such as dissolution of calcite highlighted above) from drillcores to produce a more holistic view of water-rock reaction at the SFR site.

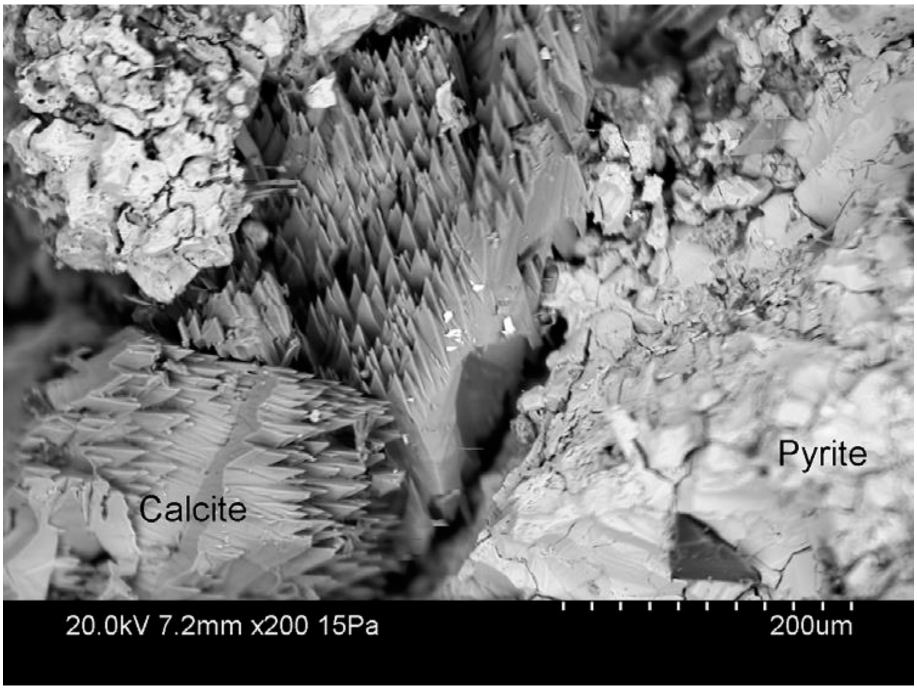

Figure 4 Backscattered electron image of calcite and pyrite crystals (from Sandström et al., 2011; page 47). Etching of calcite due to dissolution is clearly visible.

4.1.4. Degradation of grout

Although SKB recognises that degradation of cement grouts in fractures could influence groundwater composition, the Geosphere Process Report states that (SKB, 2014c; Table 5-14 on page 168):

> "*The volume of grout is relatively small compared to other cementitious materials in the SFR barriers and waste packages. Its overall contribution to the composition of SFR leachates into the geosphere is therefore neglected"*.

The summary description for this topic in the Geosphere Process Report is somewhat out of date and fails to mention modelling of grout leaching and reaction carried out by Posiva through the Long-Term Cement Studies Project (Soler, 2011) and that for the licence application for the construction of the spent fuel repository at Olkiluoto (Koskinen, 2013).

SSM should ask SKB to clarify its understanding of grout-groundwater interactions taking note of the publications identified above.

4.1.5. Salt exclusion

SFR is situated at a depth where permafrost may reach during a glacial advance and thus potentially lead to increasing salinity of groundwater through 'salt exclusion' (SKB, 2014c; Section 5.11, page 191 and following). Increased salinity of groundwater would accelerate the degradation of concrete barriers.

However these potential effects have been ruled out because (SKB, 2014c; page 192, 5th paragraph):

> "*generic simulations carried out by Vidstrand et al. (2006) suggest that a regional groundwater flow beneath a permafrost layer would cause a "flushing" of the rejected salt and hence dilute the salinity. Based on the above discussions and results, the effect of salt exclusion is considered negligible for the shallow SFR repository at Forsmark".*

The report by Vidstrand et al. (Vidstrand et al., 2006) has not been consulted for this (geochemical) study, but should be reviewed as part of the assessment of the documentation for groundwater flow by SSM.

4.2. Interaction with EBS materials

A fairly comprehensive description of the chemical interactions of the wastes with groundwater and near-field pore fluids is presented in the waste form packaging and process report (SKB, 2014e) and the EBS Process report (SKB, 2014a) for SR-PSU. These reports present thorough assessments of key issues for this topic area, although it should be noted that much of the text is common to both reports.

The durability of the cement waste form has been evaluated by long term reactive transport modelling, accounting for the coupling between dissolution-precipitation of minerals and changes in porosity, diffusivity and hydraulic conductivity, principally in the report by Höglund (Höglund, 2013).

A more simplistic assessment of the evolution of pH in SFR 1 has been reported by Cronstrand (Cronstrand, 2014) who modeled the system as a homogeneous mixing tank, and considered advective flow and thermodynamic equilibrium between different solid materials. In this latter study, with the exception of 1 BLA, the pH is predicted to be maintained above 12 throughout the initial 10,000 years. The combination of higher flow rates and low content of cement and concrete leads to a more dramatic pH evolution for BLA than the other repository parts. Cronstrand emphasises that his report is intended to be a pessimistic assessment of pH evolution.

Höglund (Höglund, 2013) provides a comprehensive description of a series of analytical and numerical reactive transport models focused on investigating physical and chemical processes that cause fractures and chemical degradation in concrete barriers, and the impact of fractures on the long term performance of SFR. The report also provides data on hydraulic conductivities, effective diffusivities and porosities of the concrete barriers, and addresses the issue of fractures in SFR barriers. This work was conducted in response to a request from SSM for further investigations of the physical and chemical concrete degradation processes that impact the concrete throughout the lifetime of the barriers. Fractures may affect several of the key parameters used in the groundwater flow modelling (hydraulic conductivity) and radionuclide transport modelling (hydraulic conductivity, effective diffusivity and sorption capability) for the SFR site. The main results presented by Höglund are:

- Fractures increase the hydraulic conductivity and effective diffusivity of the barriers. Shrinkage of the concrete, as it dries during the operational phase and cools during re-saturation with groundwater, will induce fractures.
- Fractures increase the leaching of calcium and other important chemical components from the concrete, thereby increasing the porosity of the adjacent concrete, and ultimately leading to a widening of the fractures.
- A reactive front of the potentially deleterious minerals ettringite and thaumasite that can lead to gradual deterioration of the concrete will propagate through the different concrete barriers in the period between 2,000 years and 10,000 years after closure. Chloride intrusion will cause depassivation of steel components of the barriers (reinforcement bars and form ties) and result in corrosion.
- Corrosion of reinforcement will lead to fracture formation in the concrete and spalling of the surface layer, the fractures will gradually become wider as corrosion progresses.
- Corrosion of form ties that fully penetrate the concrete walls leads to fracture formation and will eventually result in fully penetrating fractures that may extend to the edges of the concrete walls and floors.
- The barrier function will decrease with time, but the new 2BMA design will degrade much more slowly than the current 1BMA.

Höglund provides a thorough review of concrete degradation processes (chemical and physical) and has conducted extensive analytical and numerical (mainly using the PHAST code - Parkhurst et al., 2004) modeling of the interaction of concrete in the different waste vaults at SFR with different groundwater types. It is considered here that this work is a significant improvement on previous studies of this type for SFR (e.g. Gaucher et al., 2005) and addresses most of the concerns regarding concrete degradation. Clearly, there remain uncertainties regarding the degree of degradation at different timescales, but these uncertainties are discussed and evaluated by Höglund in a transparent manner.

The reaction-transport modeling carried out using PHAST (Section 7 of Höglund, 2013) considers different thermodynamic databases (MinteqCem2001 - Höglund, 2001; Cemdata07 - Matschei et al., 2007) and is thus a robust approach.

However, there are some issues which may not be safety-critical, but remain unclear nonetheless and are discussed here below.

4.2.1. Interaction with saline groundwaters

An important issue is the interaction of concrete with saline groundwater, which is envisaged to occur during the early portion of evolution of SFR (first few thousand years post-closure). The groundwater employed by Höglund in modelling studies contains 5000 mg/L chloride and (as pointed out by Höglund) is thus within the stability field of Friedel's salt, a chloride-bearing hydrated calcium aluminate ($Ca_4Al_2(OH)_{12}Cl_2(H_2O)_4$. As other authors have observed (e.g. Honda et al., 2009), the formation of Friedel's salt (e.g. from monocarboaluminate, as documented by Höglund) is accompanied by an increase in pH:

monocarboaluminate + portlandite + $2Cl^-$ →
Friedel's salt + calcite + $2OH^-$ + H_2O

Somewhat unusually, in Höglund's model results for the interaction of the various concrete barriers with saline groundwater, this reaction is not accompanied by an increase in pH, e.g. Figure 5 (below).

Another issue which is not mentioned by Höglund (Höglund, 2013) is that portlandite solubility is dependent upon salinity (see Figure 6). As stated above, the composition of groundwater selected by Höglund to represent saline conditions at SFR contains 5000 mg/L Cl^- (~ 0.14 NaCl mol/L) and would thus only slightly increase portlandite solubility according to data in Figure 6. Any underestimation of groundwater salinity would thus underestimate portlandite solubility however.

Moreover, the salinity of any ambient groundwater necessitates the selection of an appropriate model for calculation of activity coefficients for aqueous species for a cement pore water evolution model. Reardon (Reardon, 1990) used an approach employing Pitzer coefficients to tackle this issue, although Glasser et al. (Glasser et al., 1999) preferred an approach using specific interaction theory, 'SIT' (Bronsted, 1922). In his reaction-transport modelling (Section 7), Höglund has used an activity coefficient approach with either Debye-Hückel or the Davies equation which would not treat these effects of salinity on solubility in an adequate manner. The effects may be minor with Cl^- concentrations of 5000 mg/L or less, but would increase if the salinities of intruding groundwaters have been underestimated if, for example, the future upconing of saline groundwater, or the potential exclusion of salt due to freezing has been inaccurately assessed.

The stability of cement pastes in saline solutions was studied as part of the review of the Sellafield investigations of the 1990s by the UK Environment Agency, and is summarised in a report by Glasser et al. (Glasser et al., 1999). Glasser et al. found that although increasing concentrations of NaCl are not detrimental to cement performance (portlandite solubility increases with increasing NaCl content, thus increasing pH – see Figure 6 here), the presence of a $MgSO_4$ component can lead to the replacement of Ca and OH^- in the cement, forming brucite and gypsum, and resulting in an overall decrease in pH of the coexisting fluid:

$$Ca(OH)_2 + Mg^{2+} + SO_4^{2-} + 2H_2O \rightleftharpoons Mg(OH)_2 + CaSO_4.2H_2O$$

Pore fluids saturated with brucite ($Mg(OH)_2$) have a pH ~ 10 at 25 °C, in contrast with those in equilibrium with portlandite ($Ca(OH)_2$) (pH ~ 12.5).

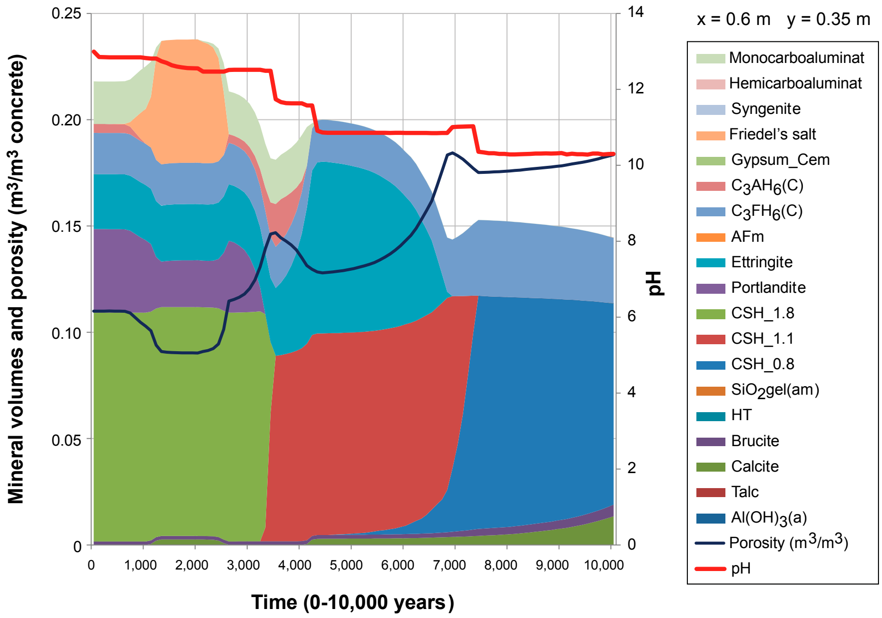

Figure 5 The change of mineral volumes and porosity in concrete during 10,000 years at position AE (a point located at the intersection of a vertical centreline through the left-hand side concrete wall and a horizontal centreline through the concrete floor). From Höglund (Höglund, 2013). Note that the replacement of monocarboaluminate by Friedel's salt and calcite between 1500 and 2500 years is not accompanied by an increase in pH which is in contrast to behaviour reported by other authors (e.g. Honda et al., 2009).

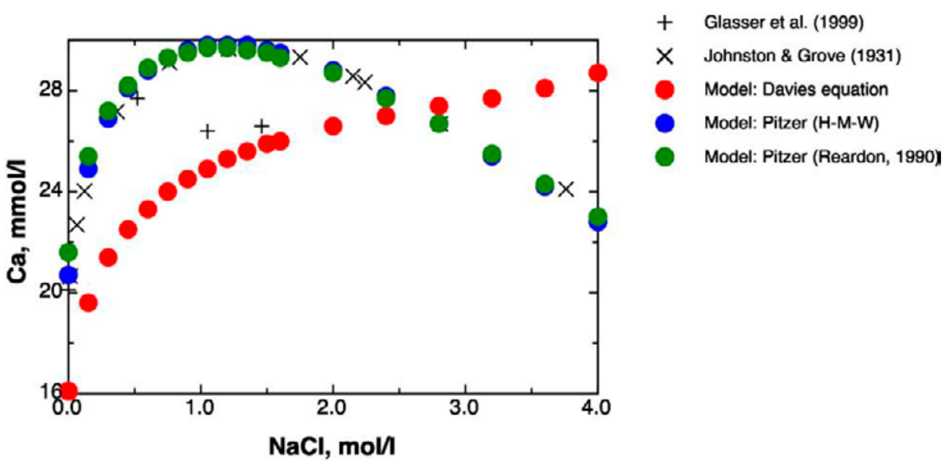

Figure 6 Comparison of predicted and measured solubility of portlandite with varying NaCl concentrations. Measured data are shown as crosses (Johnston and Grove, 1931; Glasser et al., 1999), with different aqueous speciation models shown as coloured dots. Note that the Davies model does not capture the peak in portlandite solubility at NaCl concentrations ~1 mol/L NaCl. Calculations carried out using Geochemists Workbench (Bethke, 2008) and the LLNL database 'thermo.com.V8.R6.230'.

The potentially detrimental effects of the presence of Mg^{2+} in groundwater upon pH in cement pore fluids are not highlighted by Höglund in a review of effects of groundwater (Höglund, 2013; see review of effects of groundwater on pages 33-34), but are judged as an '*important process*' at the top of page 40. The saline groundwater investigated by Höglund contains substantial amounts of both Mg^{2+} (270 mg/L; ~0.01 mol/L) and SO_4^{2-} (500 mg/L; ~0.005 mol/L) (Höglund, 2013, Table 3-1, page 29). Brucite ($Mg(OH)_2$) is less soluble than its calcic counterpart, portlandite, and buffers pore fluids at pH ~ 10. Similar reactions occur with the C-S-H gel component of the cement, with sepiolite ($Mg_4Si_6O_{15}(OH)_2{:}6H_2O$) and/or talc ($Mg_3Si_4O_{10}(OH)_2$) forming as a result. In the section on reaction-transport modelling (page 171 of Höglund, 2013) brucite is described as forming as the pH in the concrete decreases, rather than the other way around.

At high ionic strengths, anhydrite ($CaSO_4$) will form instead of gypsum ($CaSO_4.2H_2O$). In a mixed solution, Glasser et al. (1999) noted that these reactions are accelerated relative to those in either salt (NaCl, $MgSO_4$) separately. Dissolved sodium chloride enhances the solubility of both brucite and gypsum.

SSM should thus ask SKB for further clarifications regarding the interaction of cement and concrete materials with saline groundwaters, especially with regard to:

- effects of the formation of Friedel's salt upon pH;
- the impact of Mg^{2+} in groundwaters on pH; and
- the selection of models for calculation of activity coefficients of aqueous species in its modelling of concrete degradation.

4.2.2. Carbonation reactions

The analysis of leaching of concrete by groundwater presented by Höglund (Höglund, 2013; Section 5) is informative, but relies upon removal of Ca^{2+} from portlandite and/or CSH gel, and excludes carbonation effects. It is thus unclear from Höglund's analysis how 'armouring' of fractures by the formation of solid carbonates (aragonite, calcite) would impede concrete degradation and/or have deleterious effects upon radionuclide retention (decreased pore fluid pH; decreased sorption). Also, it is not clear if the exclusion of carbonation is a pessimistic assumption.

The more detailed (combined) analysis of the effects of chloride, sulphate and carbonate in Section 5.2 is more realistic, but carbonation is considered here by Höglund to consist of the formation of monocarbonate rather than calcite.

Natural analogues of cement and concrete degradation are discussed by Höglund in Section 4.1.4, but there is no mention of pertinent information from the oil industry. Cement carbonation, especially in saline solutions, is of considerable interest to the burgeoning CO_2 sequestration industry, where cement well seals are a key link in the performance of CO_2 storage systems (e.g. Wilson et al., 2011). There are numerous studies in this field, but as an example, Kutchko et al. (Kutchko et al., 2007) have described the degradation of 'Class H' cements under geological storage conditions, highlighting the occurrence of alteration zones. They report that in contact with *supercritical* CO_2, cement is converted to calcite ($CaCO_3$) at a single reaction front. In CO_2-saturated fluids, they identified three reaction zones (Figure 7) that form as a result of the following processes: portlandite ($Ca(OH)_2$) dissolution; calcite precipitation; calcite dissolution; and leaching of C-S-H gel to form amorphous silica ($SiO_{2(am)}$). The depth of alteration was found to vary as a function of cement curing conditions, with reported values ranging from 0.59 to 0.22 mm. Further analysis of these systems may be rewarding regarding the understanding of concrete degradation at SFR.

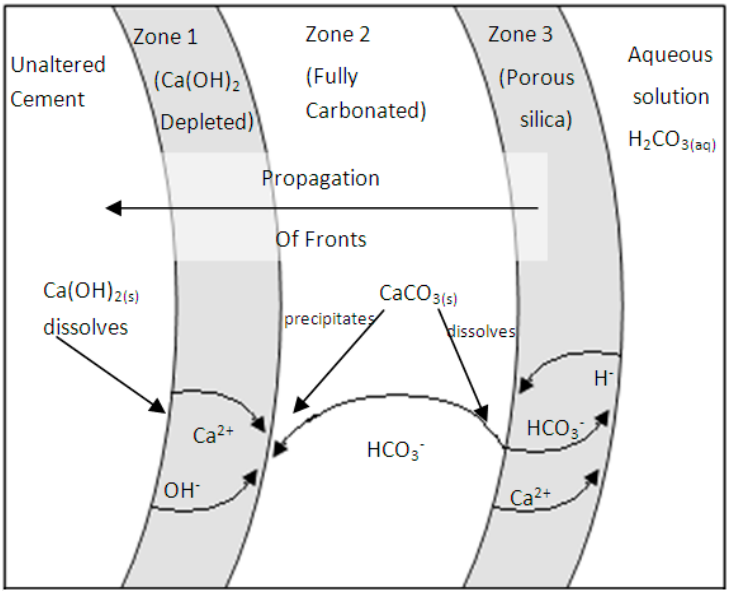

Figure 7 Schematic representation of zones of cement alteration in the experimental system of Kutchko et al. (2007) (from Wilson et al., 2011).

Moreover, such zonal structures have been observed during the carbonation of a cement backfill planned for the geological disposal of L/ILW in the UK (Rochelle et al., 2014). In the UK, concerns have been raised about 'armouring' of cement fracture surfaces by carbonation, thus lowering the ambient pH of near-field pore fluids and hindering sorption of radionuclides (e.g. Harris et al., 1997). This issue seems to have received little attention by SKB.

SSM should thus ask SKB for further clarifications regarding the interaction of cement and concrete materials with carbonate in groundwater, especially with regard to:

- the potential armouring of concrete fracture surfaces by calcite and the consequent lowering of ambient pH in the near-field; and
- Further use of natural analogues of carbonation reactions to increase confidence in the results of numerical modelling of concrete degradation.

4.2.3. Interaction with aqueous Fe^{2+} from steel corrosion

There is an in-depth discussion of the corrosion of metals in waste packages in the waste packaging process report (SKB, 2014e; Section 3.5.9, page 147 and following; Section 4.4.7, page 197 and following), but there is no discussion of the fate of ferrous iron and how it may impact upon concrete degradation in particular. This is also absent from the modelling described by Höglund (Höglund, 2013). Indeed, towards the base of page 171, it is stated:

> "*Iron is present in low concentrations in groundwater, unless the conditions are very reducing. Iron is a constituent of concrete and may appear in various minerals including iron hydroxides, hydrotalcite-Fe, iron-substituted ettringite etc. Iron also appears in large amounts in the waste and waste packaging, as well as in reinforcement and other steel construction details. Iron in the form of metal that may undergo corrosion and form dissolved or solid reactions products have not been considered in the present modelling but could be addressed in future studies*".

And again on page 251:

> "*SFR contains other steel components embedded in concrete, such as grouted waste drums and steel in concrete-conditioned waste, which is outside the scope of this report. The corrosion of these may also affect the performance of SFR and may need to be considered in future studies*".

All iron present in cement and concrete is fully oxidised to the ferric form, but under the chemically-reducing post-closure conditions of SFR, ferrous iron would be thermodynamically preferred. It is a moot point whether ferric iron in the cement could be reduced by microbiological activity associated with hydrogen released from anaerobic corrosion, but there will be substantial amounts of ferrous iron available from steel corrosion.

Consequently, it could be considered that ferrous iron derived from steel corrosion could play an important role in the degradation of cement and concrete in SFR. Although the solubility of Fe^{2+} in near-field pore fluids is limited at high pH, the inventory of iron in the repository EBS materials is large and it is conceivable that Fe^{2+} could play a similar role to that of Mg^{2+} in groundwater by substituting for Ca^{2+} in portlandite and other Ca-bearing solids. This would serve to lower the ambient pH of pore fluids from 12.5 (equilibration with portlandite) to ~9 (equilibration with $Fe(OH)_2$). This type of reaction has not been hypothesised previously, but could conceivably occur because of the very reducing conditions associated with the anaerobic corrosion of steel and likely enhanced solubility of ferrous iron.

There are concerns that the description of the process of corrosion of metal components in SFR by SKB is constrained to a large degree by reported performance of such materials in the sub-aerial (surface) environment where 'rust' (ferric oxyhydroxides of one form or another) dominates (see discussion on pages 48-49 of Höglund, 2013). It is not clear, for example, that 'rust' (or even magnetite) would form in a chemically-reducing geological environment (e.g. text on page 255 of Höglund, 2013). Consideration should therefore be given to the evaluation of how metal corrosion processes may be different in the long-term sub-surface. It may be, for example that steel corrosion is initiated under oxic conditions (e.g. before repository closure) and then proceeds anoxically. It is not clear that the large collection of published work on steel corrosion in concrete in surficial environments is relevant to deep geological disposal.

The potential interaction of Fe^{2+} from anaerobic corrosion of steel is a 'new' topic, and as such, relevant research has not been reported by other waste management agencies. Nevertheless, this issue could potentially have a large impact upon concrete degradation processes and near-field pH so that SSM needs to ask SKB what it plans to do about the issue in its future R&D programme.

4.2.4. Saturation of bentonite in the Silo

SKB discusses saturation of bentonite in the Silo in Section 7.4.1 of the EBS Process Report (SKB, 2014a, page 200 and following). In this discussion, reference is made to a number of experimental studies describing evidence for uptake of water (saturation), both in the laboratory (e.g. Karnland et al., 2006) and in the LOT field tests at Äspö (e.g. Karnland et al., 2009). However, it should be noted that none of these studies refer to saturation with cement/concrete pore water which would be the case in the Silo. Indeed there are no reported studies anywhere of saturation of bentonite with water conditioned with cement (see Savage, 2009). It is not clear how saturation of bentonite with cement pore water would affect its swelling properties.

SSM should ask SKB for clarification of this issue.

5. Inclusion of effects in TR-14-01

5.1. Natural Evolution of the Site

Text in TR-14-01 re-iterates that SFR groundwaters show a narrow range of chloride variation (1500 to 5500 mg/L Cl^-) compared with the Forsmark site (50 to 16000 mg/L Cl^-). Furthermore, 'marine indicators', such as Mg/Cl, K/Cl and Br/Cl ratios also show relatively large variations, especially considering the limited salinity range. SKB believes that this suggests the presence of groundwaters with different origins. Groundwaters are weakly reducing (−140 to −190 mV) with redox-buffering capacity consisting of fracture-filling iron(II) minerals which cover the conductive fractures. In SFR, these consist mainly of chlorite, clay minerals and pyrite. Four groundwater types are defined with characteristic features, reactions, and origins (Table 1).

SKB states that measurement series in boreholes and tunnel systems at SFR show that the chloride content of groundwaters declined between years 1986 and 2000, followed by a nearly stable period up to year 2010 (SKB, 2014d; page 126, 3rd paragraph). SKB sees this as expected behaviour, since the greatest changes with regard to groundwater pressure and inflows to the boreholes and the tunnel system occurred soon after construction. During the construction and operation of SFR 3, SKB expects mainly the same evolution in groundwater chemistry as in SFR 1, with an increasing occurrence of the local Baltic Sea and Mixed transition groundwater types.

SKB considers that the water in the repository during its initial state will be the brackish-type (Table 1) and interaction with cementitious barriers will contribute to an increase of the pH in the water in the repository. During the sampling period 1986 to 2010, SKB observed a slightly increasing trend in the groundwater pH, but the range of measured values was large. Moreover, SKB believes that predictability with regard to the expected composition of the groundwater is good, and it is improbable that any extreme water compositions other than those already encountered will be discovered during the construction phase. However, two significant uncertainties are:

- there are no baseline hydrochemical data prior to the construction of SFR (SKB, 2014d; page 127, 2nd paragraph).
- There are no data from boreholes deeper than 400 m at the SFR site.

Table 1 Groundwater types in SFR – composition, reactions/processes and origin. From SKB (SKB, 2014d).

Groundwater type	Composition/ characteristics	Dominant reactions and processes	Origin
Local Baltic	Chloride 2,500–3,500 mg/L $\delta^{18}O$ −9 to −7.5‰ V-SMOW Na-(Ca)-(Mg)-Cl-SO_4 type Cl/Mg weight ratio < 27	Ion exchange and micro-biological reactions in the bedrock have resulted in decreased concentrations of Mg, K, Na and SO_4^{2-} as well as enrichment of Ca and HCO_3^- compared with Baltic Sea water.	It is unclear whether the Baltic Sea water was present at all in the deformation zones before the construction of the tunnels in SFR. It is more probably a modern component that has been introduced due to the drawdown caused by tunnels.
Littorina with a glacial component	Chloride 3,500–6,000 mg/L $\delta^{18}O$ −9.5 to −7.5 ‰ V-SMOW Na-Ca-(Mg)-Cl-SO_4 type Cl/Mg weight ratio < 27	The Na/Ca ratio is lower than the marine ratio. These changes are caused by ion exchange, but also by dilution with glacial meltwater.	Compared with the original Littorina water, it has been diluted (lower Cl and $\delta^{18}O$ values) with glacial meltwater.
Brackish-glacial	Chloride 1,500–5,000 mg/L $\delta^{18}O$ < −12.0 ‰ V-SMOW Na-Ca-Cl type Cl/Mg weight ratio > 32	An old mixture of different, mainly non-marine ground-waters.	This is the oldest groundwater type and the amounts of post-glacial components are very small. It is a mixture of primarily glacial meltwater (last deglacia-tion or older) and brackish non-marine water (pre-glacial). It probably contains components of old meteoric water prior to last deglaciation as well.
Mixed-brackish (transition type)	Chloride 2,500–6,000 mg/L $\delta^{18}O$ −12.0 to −9.5‰ V-SMOW Na-Ca-(Mg)-Cl-(SO_4) type	Natural or artificial mixing of the three different ground-water types above.	Significant mixing of the brackish- glacial and the two brackish marine groundwater types (mostly the Littorina type) has caused this ground water of transition type. It is more common during the last two decades, according to data from long time series which suggests artificial mixing due to the presence of the repository.

Potential perturbation of groundwater compositions due to periglacial conditions has been ruled out for SFR (TR-14-01), towards foot of page 200):

> "*Based on currently available hydrogeochemical information, the groundwater expected to be present around the repository during periods of a periglacial climate domain will be similar to the waters expected during the temperate domain under terrestrial conditions, when the repository is not covered by the sea (see the chosen groundwater composition in Table 6-8). Freeze-out of constituents dissolved in the groundwater can increase the salinity of the liquid phase. Although somewhat dependent of the timing of this period, the effect of such a process is not expected to have any major impact on the salinity distribution in a groundwater that will be substantially diluted by meteoric water at that time*".

It is considered here that the rationale for this perspective should be reconsidered as part of the review by SSM.

'Favourable water chemistry' is identified as an important feature for the engineered barrier/groundwater system in that sorption (of radionuclides) is heavily dependent on the composition of the pore water (SKB, 2014d; top of page 135). The most important parameters are deemed to be pH, redox potential, and the concentrations of complexing agents. pH is desired to be higher than 10.5 which generally guarantees favourable sorption conditions for important cations. Anions are assumed to sorb poorly to cementitious materials in the entire relevant pH range. A low redox potential leads to a slower release of important radionuclides.

Consequently, 'good retention' has been defined as a safety function for the EBS, with the following safety function indicators (SKB, 2014d; Table 5-3, page 137):

- pH in concrete barriers (1–2BMA, 1–2BTF, silo, BRT),
- redox potential in concrete barriers (1–2BMA, 1–2BTF, silo, BRT),
- concentrations of complexing agents in concrete barriers (1–2BMA, 1–2BTF, silo),
- available specific surface area for sorption in concrete barriers (1–2BMA, 1–2BTF, silo, BRT).

The chemically-relevant aspect of the geosphere is 'good retention', which is controlled by reducing conditions at repository depth. The relevant safety function indicator is:

- redox potential.

Geochemical evolution of the SFR repository system is discussed in Section 6.3.6 of TR-14-01 and is firmly linked with climatic and shoreline changes shifting groundwater flow patterns. The brackish groundwater type has been chosen as the reference composition of the first 1000 years of evolution with high pH conditions from the degradation of the engineered barriers affecting downstream from the repository. SKB goes onto state (SKB, 2014d; top of page 154):

> "*The durability of the near-field system is highly dependent of the longevity of the engineered barriers in the repository as they are affected by chemical reactions that take place when the barriers come into contact with the groundwater and waste. The chemical evolution of the barriers is also of importance for sorption and for the release of radionuclides and other species*".

Redox is viewed by SKB to be of high importance in the safety assessment (bottom of page 159 of TR-14-01) and SKB considers that if the system responds to the Fe-magnetite system, and considering the evolution of pH due to degradation of the concrete barriers, the redox potential would be about –0.7 V at pH =12.5. This could be achieved within 5 years of repository closure. Redox evolution in SFR is discussed in detail in a paper by Duro et al. (Duro et al., 2014). This paper presents a rigorous and thorough investigation of the issue. They consider that corrosion of the steel-based material present in the repository keeps the system under reducing conditions for long time periods. Their simulations considered both the presence and the absence of microbial activity. In the initial stages after the repository closure, they found that the microbially-mediated oxidation of organic matter rapidly causes the depletion of oxygen in the system. The system is thereafter kept under reducing conditions, and hydrogen is generated due to the anoxic corrosion of steel. The times for exhaustion of the steel contained in the vaults vary from 5 ka to more than 60 ka in the different vaults, depending on the amount and the surface area of steel. After the complete corrosion of steel, they believe that the system would still maintain a high reducing capacity, due to the magnetite formed as a steel corrosion product. Simulations assuming presence of oxic water due to glacial melting, intruding the system 60 ka after repository closure, indicate that magnetite is progressively oxidised, forming Fe(III) oxides. The time at which magnetite is completely oxidised varies depending on the amount of steel initially present in the waste package.

However, it should be noted that there is uncertainty regarding magnetite being the 'end-point' of anaerobic corrosion of steel at low temperatures. Some authors (e.g. Reardon, 1995; Wilkin et al., 2003; Phillips et al., 2000) believe that the transformation of $Fe(OH)_2$ (initial corrosion product) to magnetite (theoretical long-term corrosion product) is unlikely at temperatures less than 100 °C. This would imply much higher concentrations of Fe^{2+} in the near-field due to buffering by $Fe(OH)_2$ solubility with the potential for its substitution for Ca^{2+} in Ca-hydroxides and C-S-H, thus lowering the long-term pH of the near-field. This uncertainty is not acknowledged by Duro et al. (Duro et al., 2014) or elsewhere in the SR-PSU documentation.

Of course, the attainment of such reducing conditions in the repository implies a sharp redox front with the geological barrier where the redox state may be maintained at the relatively more oxidizing conditions of hematite-magnetite equilibrium. Therefore, chemically-reducing fluids (containing hydrogen and organic acids) migrating from the repository will tend to destabilize redox-sensitive mineral such as Fe-oxides and clays in the geosphere. This issue is not addressed in documentation for SR-PSU.

There are a number of issues from the above text that should be further investigated:

- the rationale for the omission of the potential perturbation of groundwater compositions due to periglacial conditions should be reconsidered as part of the detailed review by SSM.
- Further information from SKB should be obtained regarding its rationale for assuming that magnetite would be the end-point for steel corrosion when strong evidence suggests that this mineral should be metastable under SFR conditions.
- As suggested earlier in this review, SKB should be asked to include the potential interaction of Fe^{2+} from anaerobic corrosion with Ca-bearing solids in cement and concrete in its future R&D programme.

5.2. Evolution of the Engineered Barrier System

Text regarding concrete degradation in TR-14-01 (page 171 and following; page 194 and following) is reliant upon the thorough evaluation of Höglund (Höglund, 2013). As discussed above, this is a much-improved analysis over that described by Gaucher et al. (Gaucher et al., 2005) with a more complete treatment of cement dissolution-precipitation processes. However, there is no cross-reference with the calculations performed by Cronstrand (Cronstrand, 2014, see paragraph here below) regarding pH evolution in the concrete barriers.

Text in TR-14-01 uses that from Cronstrand's modelling (Cronstrand, 2014) to describe the evolution of pH within the cement barriers (SKB, 2014d; towards foot of page 189). This assumes that the pH will stay at approximately 12.5, corresponding to buffering by portlandite dissolution in all waste domains, except for 1BLA, in SFR 1 for at least 100 ka.

The 'accelerated concrete degradation scenario' (TR-14-01, Section 7.6.3, page 233) utilises the modeling of Höglund (2014) which describes physical degradation (changes in diffusivity and porosity) of the concrete with time and assumes that the hydraulic conductivity of the concrete increases earlier than in the main scenario. However, this accelerated physical degradation is not accompanied in this scenario by accelerated chemical degradation. SKB assumes that the long-term evolution of the flow-limiting ability of the concrete structure is associated with a transformation of cement minerals, and the flow-limiting function is maintained for at least 20 000 years (Höglund, 2014 and Chapter 6 of TR-14-01).

5.3. Responses to Comments from SSM on SAR-08

Overall, SKB has addressed many of the concerns raised by SSM through the review of SAR-08 regarding the chemical evolution of groundwater and near-field pore fluids. As documented in TR-14-01, these concerns are:

- **Chemical evolution of the near-field**. The persistence of chemically-reducing conditions in the repository and the possibility that conditions could become oxic in the long-term (TR-14-01, Section 3.9.2, page 453). In response, SKB has now modelled the probable redox development in SFR 1 after closure (Duro et al., 2014). Based on this modelling, the probability of future oxidising conditions has been assessed. Furthermore, the consequences of oxidising conditions, e.g. changed speciation of redox-sensitive nuclides, are assessed as part of SKB's response to SSM's suggestions concerning the risk and consequences of changing redox conditions at repository depth. *Nevertheless, the review carried out here describes a previously undocumented (redox-related) uncertainty that has not been considered in SR-PSU, which is the potential role of ferrous iron from anaerobic corrosion of steel and its potential effect upon cement and concrete degradation through its likely substitution for* Ca^{2+} *ions in hydrated cement solids such as portlandite and C-S-H gel and its consequent impact upon pH evolution and sorption characteristics of the altered cement/concrete.*
- **Degradation of engineered barriers**. In SR-PSU, SKB has extended the assessment of long-term barrier evolution, and concluded that barrier degradation can be expected to occur earlier than was estimated in SAR-08. In its modelling for SR-PSU, SKB has accounted for gradual barrier degradation over time in the main scenario, as explained in Section 7.4.3 of the TR-14-01. The main scenario is complemented by the scenario 'Accelerated concrete degradation' (TR-14-01, Section 7.6.3) and the scenario 'Loss of barrier function – high flow in the repository' (TR-14-01, Section 7.7.3) to further improve the understanding of how the degradation

of concrete barriers affects the performance of the repository. This is in response to SSM's view that SKB's approach for taking degradation of barriers and tunnel plugs into account being the same as in FSR 2001, when the consequence analysis calculations were based on an instantaneous increase of hydraulic conductivity in relevant repository components by several powers of ten. SSM's view of this aspect of SAR-08 is that the method is simple but provides no basis for assessment of the expected gradual and heterogeneous course of barrier degradation. Since no barrier changes are included in the main scenario for a period up to 40,000 years, SSM stated that it could not exclude the possibility that this is an optimistic rather than a conservative case. The review presented here shows that SKB has significantly improved its approach to barrier degradation, principally through the study by Höglund (2013), but that this approach could be extended to consider the effects of the presence of more saline groundwaters.

6. Conclusions and Summary

This document provides a review of the chemical evolution in rock and engineered barrier systems as described in the SR-PSU documentation. The review has been conducted with regard to:

- Completenesss.
- Scientific soundness and quality.
- Adequacy of relevant models, data and safety functions.
- Handling of uncertainties.
- Safety significance.
- Quality in terms of transparency and traceability of information.
- Feasibility of manufacturing, construction, testing, implementation and operation.

It is concluded from this initial review that for the most part, there is a good assessment of the characteristics, influences and uncertainties for the evolution of the site and engineered barriers regarding potential salinity changes, pH, and Eh in SR-PSU documentation. However, there are some issues which require further attention, either by SKB and/or SSM. These have been grouped accordingly below.

6.1. Complementary Information Requirements from SKB

The following topics/issues require additional information from, and consideration by, SKB:

- An understanding of how the rock-groundwater system has responded to environmental changes in the past is a key issue in forecasting future behaviour. SKB should be encouraged to carry out sampling of matrix pore waters in its future activities at the SFR site.
- There is an incomplete presentation of principal component analysis (PCA) for groundwaters at the SFR site, with data only for Cl^-, $\delta^{18}O$, δ^2H and SO_4 being presented by SKB to determine mixing relationships. A full dataset would allow an evaluation of the role of water-rock reactions in the past and future evolution of groundwaters at the site. SKB should carry out a more detailed PCA study of SFR groundwaters, investigating more groundwater species than published thus far.
- SSM should ask for further clarification from SKB regarding the links between the oxidation of organic matter and the reduction of sulphate in groundwaters at SFR. This reaction could be a key control of redox in the far-field (thus influencing radionuclide solubility and sorption).
- SSM should ask SKB why the presence of saline groundwater at repository levels by up-coning from depth was not considered as an 'unlikely scenario' in the SR-PSU assessment.
- SKB should be asked to offer explanations as to why there are marked differences between the composition of clay minerals at the SFR and Forsmark sites, despite (apparently) similar histories of water-rock reaction.
- SSM should ask SKB to clarify its understanding of redox in groundwaters at SFR, especially the link between measured Eh values in groundwater and the presence of redox-sensitive minerals (Fe-oxides, clays) in rock

fractures. SKB's current interpretation is at best vague, and at worst, highly uncertain.

- SSM should ask SKB to clarify its understanding of grout-groundwater interactions taking note of previous publications on this topic not referred to in SR-PSU documentation.
- SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with saline groundwaters, especially with regard to:
    - effects of the formation of Friedel's salt upon pH;
    - the impact of Mg^{2+} in groundwaters on pH; and
    - the selection of models for calculation of activity coefficients of aqueous species in its modelling of concrete degradation.
- SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with carbonate in groundwater, especially with regard to:
    - the potential armouring of concrete fracture surfaces by calcite and the consequent lowering of ambient pH in the near-field; and
    - Further use of natural analogues of carbonation reactions to increase confidence in the results of numerical modelling of concrete degradation.
- The potential interaction of Fe^{2+} from anaerobic corrosion of steel with cement and concrete is a 'new' topic, and as such, relevant research has not been reported by other waste management agencies. Nevertheless, this issue could potentially have a large impact upon concrete degradation processes and near-field pH so that SSM needs to ask SKB what it plans to do about the issue in its future R&D programme.
- SSM should ask SKB for clarification of the issue of how bentonite might have resaturated with cement pore fluids in the Silo.

6.2. Topics for Detailed Review by SSM

The following topics/issues are suggested for inclusion in the detailed review stage of the review of SR-PSU by SSM:

- SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB. This study should attempt to link observations of groundwater chemistry and mineralogical evidence from drillcores to produce a more holistic view of water-rock reaction at the SFR site.
- A re-evaluation of the potential for up-coning of saline groundwater from depth should be carried out to confirm SKB's conclusions on this issue.
- The report by Vidstrand et al. (Vidstrand et al., 2006) on the exclusion of the effects of salt exclusion during periglacial conditions should be reviewed to assess the validity of SKB's conclusion that any occurrence of salt exclusion in the past would have been flushed from the rock-groundwater system.
- The effects of saline groundwater on concrete degradation should be modelled to assess rates of degradation and potential changes to pH.

7. References

Andrews, J. E., Brimblecombe, P., Jickells, T. D., and Liss, P. S., An Introduction to Environmental Chemistry, Blackwell Science, Oxford, UK, 1996.

Bethke, C. M., Geochemical and Biogeochemical Reaction Modeling, Cambridge University Press, Cambridge, UK, 2008.

Bronsted, J. N., *Studies on solubility; IV. The principle of the specific interaction ions*. Journal of the American Chemical Society 44**:** 877-898, 1922.

Coudrain-Ribstein, A., Gouze, P., and de Marsily, G., *Temperature-carbon dioxide partial pressure trends in confined aquifers*. Chemical Geology 145**:** 73-89, 1998.

Cronstrand, P., *Modelling the long-time stability of the engineered barriers of SFR with respect to climate changes,* SKB Report R-07-51, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2007.

Cronstrand, P., *Evolution of pH in SFR 1,* SKB Report R-14-01, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2014.

Duro, L., Domènech, C., Grivé, M., Roman-Ross, G., Bruno, J., and Källström, K., *Assessment of the evolution of the redox conditions in a low and intermediate level nuclear waste repository (SFR1, Sweden)*. Applied Geochemistry 49**:** 192-205, 2014.

Gaucher, E. C., Tournassat, C., and Nowak, C., *Modelling the geochemical evolution of the multi-barrier system of the Silo of the SFR repository,* SKB Report R-05-80, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2005.

Gieskes, J. M., and Lawrence, J. R., *Alteration of volcanic matter in deep-sea sediments: evidence from the chemical composition of interstitial waters from deep-sea drilling cores*. Geochimica et Cosmochimica Acta 45**:** 1694, 1981.

Gimeno, M. J., Auqué, L. F., Gomez, J. B., and Acero, P., *Site investigation SFR Water-rock interaction and mixing modelling in the SFR,* SKB Report P-11-25, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2011.

Glasser, F. P., Tyrer, M., Quillin, K., Ross, D., Pedersen, J., Goldthorpe, K., Bennett, D., and Atkins, M., *The chemistry of blended cements and backfills intended for use in radioactive waste disposal,* R&D Technical Report P98, UK Environment Agency, 1999.

Harris, A. W., Atkinson, A., Cole, G. B., Haworth, A., Nickerson, A. K., and Smith, A. C., *The performance of cementitious barriers in repositories,* Nirex Safety Studies Report NSS/R389, UK Nirex Limited, Harwell, UK, 1997.

Höglund, L., *Project SAFE. Modelling of long-term concrete degradation processes in the Swedish SFR repository,* SKB Report R-01-08, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2001.

Höglund, L., *The impact of concrete degradation on the BMA barrier functions,* SKB Report R-13-40, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2013.

Honda, A., Masuda, K., Nakanishi, H., Fujita, H., and Negishi, K.: Modeling of pH elevation due to the reaction of saline groundwater with hydrated ordinary Portland cement phases. *In* Scientific Basis for Nuclear Waste Management.

Johnston, J., and Grove, C., *The solubility of calcium hydroxide in aqueous salt solutions*. Journal of the American Chemical Society 53**:** 3976-3991, 1931.

Karnland, O., Olsson, S., Dueck, A., Birgersson, M., Nilsson, U., Hernan-Hakansson, T., Pedersen, A. K., Nilsson, S., Eriksen, T. E., and Rosborg, B., *Long term test of buffer material at the Äspö Hard Rock Laboratory, LOT project. Final report on the A2 test parcel,* SKB Report TR-09-29, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2009.

Karnland, O., Olsson, S., Nilsson, U., and Sellin, P., *Mineralogy and sealing properties of various bentonites and smectite-rich clay materials,* SKB Technical Report TR-06-30, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2006.

Kastner, M., Elderfield, H., Martin, J. B., Suess, E., Kvenvolden, K. A., and Garrison, R. E.: Diagenesis and interstitial water chemistry at the Peruvian continental margin: major constituents and strontium isotopes. *In* Proceedings of the Ocean Drilling Program, Scientific Results, pp. 413-440.

Koskinen, K., *Effects of cementitious leachates on the EBS,* Posiva Report 2013-04, Posiva Oy, Eurajoki, Finland, 2013.

Kutchko, B. G., Strazisar, B. R., Dzombak, D. A., Lowry, G. V., and Thaulow, N., *Degradation of well cement by CO_2 under geological sequestration conditions*. Environmental Science and Technology 41**:** 4787-4792, 2007.

Matschei, T., Lothenbach, B., and Glasser, F. P., *Thermodynamic properties of Portland cement hydrates in the system CaO-Al_2O_3-SiO_2-$CaSO_4$-$CaCO_3$-H_2O*. Cement and Concrete Research 37**:** 1379-1410, 2007.

Moore, G. F., Taira, A., Klaus, A., Becker, K., Becker, L., Boeckel, B., Cragg, B. A., Dean, P. A., Fergusson, C. L., Henry, P., Hirano, S., Hisamitsu, T., Hunze, S., Kastner, M., Maltman, A. J., Morgan, J. K., Murakami, Y., Saffer, D. M., Sánchez-Gómez, M., Screaton, E. J., Smith, D. C., Spivack, A. J., Steurer, J., Tobin, H. J., Ujiie, K., Underwood, M. B., and Wilson, M., *Deformation and fluid flow processes in the Nankai Trough accretionary prism, covering Leg 190 of the cruises of the Drilling Vessel JOIDES Resolution Sydney, Australia, to Yokohama, Japan Sites 1173–1178 6 May–16 July 2000,* Volume 190 Initial Reports, Ocean Drilling Program, 2001.

Nilsson, A.-C., Tullborg, E.-L., Smellie, J. A. T., Gimeno, M., Gomez, J., Auqué, L. F., Sandström, B., and Pedersen, A. K., *SFR site investigation Bedrock Hydrogeochemistry,* SKB Report R-11-06, Swedish Nuclear Fuel and Waste Management Co, Stockholm, Sweden, 2011.

Parkhurst, D. L., Kipp, K. L., Engesgaard, P., and Charlton, S. R., *PHAST - A program for simulating ground-water flow, solute transport, and multicomponent geochemical reactions,* Techniques and Methods 6-A8, US Geological Survey, 2004.

Phillips, D. H., Gu, B., Watson, D. B., Roh, Y., Liang, L., and Lee, S. Y., *Performance evaluation of a zerovalent iron reactive barrier: mineralogical characterisitics*. Environmental Science and Technology 34**:** 4169-4176, 2000.

Reardon, E. J., *An ion interaction model for the determination of chemical equilibria in cement/water systems*. Cement and Concrete Research 20**:** 175-192, 1990.

Reardon, E. J., *Anaerobic corrosion of granular iron: measurement and interpretation of hydrogen evolution rates*. Environmental Science and Technology 29**:** 2936-2945, 1995.

Rochelle, C. A., Purser, G., Milodowski, A. E., and Wagner, D., *Results of laboratory carbonation experiments on Nirex Reference Vault Backfill cement,* British Geological Survey Open Report OR/14/014, British Geological Survey, Keyworth, UK, 2014.

Sandström, B., Nilsson, K., and Tullborg, E.-L., *Site Investigation SFR. Fracture mineralogy including identification of uranium phases and hydrochemical characterisation of groundwater in borehole KFR106,* SKB Report P-11-41, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2011.

Sandström, B., and Tullborg, E.-L., *Site investigation. SFR Fracture mineralogy and geochemistry of borehole sections sampled for groundwater chemistry and Eh. Results from boreholes KFR01, KFR08, KFR10, KFR19, KFR7A and KFR105,* SKB Report P-11-01, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2011.

Sandström, B., Tullborg, E.-L., Smellie, J. A. T., Mackenzie, A. B., and Suksi, J., *Fracture mineralogy of the Forsmark site. SDM-Site Forsmark,* SKB Report R-08-102, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2008.

Savage, D., *A review of experimental evidence for the development and properties of cement-bentonite Interfaces with implications for gas transport,* Nagra Report NAB 09-30, Nagra, Wettingen, Switzerland, 2009.

Savage, D., *Geochemical constraints on buffer pore water evolution and implications for erosion. In: 'Copper Corrosion and Buffer Erosion'. Synthesis and Extended Abstracts from a Workshop in Stockholm, Sweden, September 15-17, 2010,* SSM Report 2011:08, Swedish Radiation Safety Authority, Stockholm, Sweden, 2011.

Savage, D., *Initial review of chemical and erosional processes within the buffer and backfill - geochemical processes,* SSM Technical Note 2012:28, Swedish Radiation Safety Authority, Stockholm, Sweden, 2012.

Savage, D., and Arthur, R., *pH and* PCO_2 *in groundwaters in fractured hard rocks*, In (J. Hendry, P. Carey, J. Parnell, A. Ruffell, and R. Worden eds) Geofluids II '97, The Queen's University Belfast, Belfast, Northern Ireland, 1997.

Savage, D., Arthur, R. C., and Saito, S.: Geochemical factors in the selection and assessment of sites for the deep disposal of radioactive wastes. *In* Chemical Containment of Wastes, pp. 27-45.

Savage, D., Arthur, R. C., Saito, S., and Morooka, K.: Water-rock buffering of pH and redox and consequences for the performance of the far-field barrier. *In* Radioactive Waste Management and Environmental Radiation, Nagoya, Japan.

Savage, D., Bateman, K., Milodowski, A. E., and Hughes, C. R., *An experimental evaluation of the reaction of granite with streamwater, seawater and NaCl solutions at 200°C*. Journal of Volcanology and Geothermal Research 57**:** 167-191, 1993.

Sayles, F. L., *The composition and diagenesis of interstitial solutions: I. Fluxes across the seawater-sediment interface in the Atlantic Ocean*. Geochimica et Cosmochimica Acta 43**:** 527-545, 1979.

SKB, *Site description of the SFR area at Forsmark at completion of the site investigation phase SDM-PSU Forsmark,* SKB Report TR-11-04, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2011.

SKB, *Engineered barrier process report for the safety assessment SR-PSU,* SKB Report TR-14-04, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2014a.

SKB, *FEP report for the safety assessment SR-PSU,* SKB Report TR-14-07, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2014b.

SKB, *Geosphere process report for the safety assessment SR-PSU,* SKB Report TR-14-05, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2014c.

SKB, *Safety analysis for SFR. Main report for the safety assessment SR-PSU,* SKB Report TR-14-01, Swedish Nuclear Fuel and Waste Management Company, Srockholm, Sweden, 2014d.

SKB, *Waste form and packaging process report for the safety assessment SR-PSU,* SKB Report TR-14-03, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2014e.

Soler, J. M., *Reactive transport modelling of grout-water interaction in a fracture at the ONKALO site - Effect of different potential groundwater compositions,* Posiva Working Report 2011-83, Posiva Oy, Eurajoki, Finland, 2011.

Vidstrand, P., Svensson, U., and Follin, S., *Simulation of hydrodynamic effects of salt rejection due to permafrost. Hydrogeological numerical model of density-driven mixing, at a regional scale, due to a high salinity pulse. SKB* SKB Report R-06-101, Swedish Nuclear Fuel and Waste Management Company, Stockholm, Sweden, 2006.

Wilkin, R. T., R.W., P., and Sewell, G. W., *Long-term performance of permeable reactive barriers using zero-valent iron: geochemical and microbiological effects*. Groundwater 41**:** 493-503, 2003.

Wilson, J. C., Benbow, S. J., Metcalfe, R., Savage, D., Walker, C. S., and Chittenden, N., *Fully coupled modeling of long term cement well seal stability in the presence of* CO_2. Energy Procedia 4**:** 5162-5169, 2011.

APPENDIX 1

Coverage of SKB reports

The following reports have been covered in the review.

Table A:1

Reviewed report	Reviewed sections	Comments
TR-14-01, Safety analysis for SFR Long-term safety Main report for the safety assessment SR-PSU (SKB)	All main sections read	The main report for the assessment SR-PSU.
TR-14-03, Waste form and packaging process report for the safety assessment SR-PSU (SKB)	Chapters 3.5, 4.4	Much of text is the same as in TR-14-04. State of the art descriptions for chemical evolution.
TR-14-04, Engineered Barrier Process Report for the Safety Assessment SR-PSU (SKB)	Chapters 5.4, 6.4, 7.4, 8.4, 9.4, 10.4	Much of text is the same as in TR-14-03. State of the art descriptions for chemical evolution.
TR-14-07, FEP report for the safety assessment SR-PSU (SKB)	Scanned for relevant FEPs	Many of the relevant FEPs are very broad in scope and do not consider specific interactions of relevance
TR-11-04, Site description of the SFR area at Forsmark at completion of the site investigation phase SDM-PSU Forsmark (SKB)	Chapter 8	The main description of the geological and hydrogeological conditions at the SFR site. Hydrogeochemical data are somewhat spatially-limited both in areal and depth terms. Interpretations are strongly based on those developed for the Forsmark site.
R-11-06, SFR site investigation bedrock hydrogeochemistry (*A-C. Nilsson et al.)*	Key sections read, but not reviewed in detail	The most detailed hydrogeochemical description for SR-PSU. Interpretations are based mainly upon the mixing of 4 groundwater types.
P-11-25, Site investigation SFR Water-rock interaction and mixing modelling in the SFR (*M. Gimeno et al.*)	Key sections read, but not reviewed in detail	Modelling of hydrogeochemicall data. Strong emphasis upon mixing rather than water-rock interaction, despite its title.
R-08-102, Fracture mineralogy of the Forsmark site, SDM-Site Forsmark (*B. Sandström et al.*)	Key sections read, but not reviewed in detail	Fracture mineral data for the Forsmark site.
P-11-01, Site investigation. SFR Fracture mineralogy and	Key sections read, but not reviewed in	The main dataset for the mineralogical compositions of

geochemistry of borehole sections sampled for groundwater chemistry and Eh. Results from boreholes KFR01, KFR08, KFR10, KFR19, KFR7A and KFR105 (*B. Sandström & E-L. Tullborg*)	detail	fractures at SFR showing that clay minerals like mixed layer illite-smectite and illite dominate in contrast to Forsmark where corrensite dominates.
TR-14-05, *Geosphere process report for the safety assessment SR-PSU,* (SKB)	Chapter 5	A description of natural processes affecting chemical evolution of groundwater at the SFR site. This report has a more balanced assessment of the role of different processes than that presented in TR-11-04, R-11-06 and P-11-25.
R-13-40, T*he impact of concrete degradation on the BMA barrier functions (L. Höglund)*	All main text sections reviewed, but not Appendices	A thorough and comprehensive analysis of physical and chemical degradation processes in concrete at SFR, but there are some omissions/uncertainties regarding salinity effects, carbonation, and the role of ferrous iron from steel corrosion in concrete degradation *inter alia*. Doesn't include interactions with waste materials, but R-14-01 below, does.
R-14-01, Evolution of pH in SFR 1 (*P. Cronstrand*)	Text read for comparison with modelling presented in R-13-40	A more simplistic and pessimistic modelling study as compared with R-13-40, treating the near-field as a mixing tank and dealing with advection and equilibrium reactions only. No reference to the R-13-40 report.

APPENDIX 2

Suggested needs for complementary information from SKB

1. An understanding of how the rock-groundwater system has responded to environmental changes in the past is a key issue in forecasting future behaviour. SKB should be encouraged to carry out sampling of matrix pore waters in its future activities at the SFR site.
2. There is an incomplete presentation of principal component analysis (PCA) for groundwaters at the SFR site, with data only for Cl^-, $\delta^{18}O$, δ^2H and SO_4 being presented by SKB to determine mixing relationships. A full dataset would allow an evaluation of the role of water-rock reactions in the past and future evolution of groundwaters at the site. SKB should carry out a more detailed PCA study of SFR groundwaters, investigating more groundwater species than published thus far.
3. SSM should ask for further clarification from SKB regarding the links between the oxidation of organic matter and the reduction of sulphate in groundwaters at SFR. This reaction could be a key control of redox in the far-field (thus influencing radionuclide solubility and sorption).
4. SSM should ask SKB why the presence of saline groundwater at repository levels by up-coning from depth was not considered as an 'unlikely scenario' in the SR-PSU assessment.
5. SSM should ask SKB to clarify its understanding of redox in groundwaters at SFR, especially the link between measured Eh values in groundwater and the presence of redox-sensitive minerals (Fe-oxides, clays) in rock fractures. SKB's current interpretation is at best vague, and at worst, highly uncertain.
6. SSM should ask SKB to clarify its understanding of grout-groundwater interactions taking note of previous publications on this topic not referred to in SR-PSU documentation.
7. SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with saline groundwaters, especially with regard to:
    a. effects of the formation of Friedel's salt upon pH;
    b. the impact of Mg^{2+} in groundwaters on pH; and
    c. the selection of models for calculation of activity coefficients of aqueous species in its modelling of concrete degradation.
8. SSM should ask SKB for further clarifications regarding the interaction of cement and concrete materials with carbonate in groundwater, especially with regard to:

    a. the potential armouring of concrete fracture surfaces by calcite and the consequent lowering of ambient pH in the near-field; and
    b. Further use of natural analogues of carbonation reactions to increase confidence in the results of numerical modelling of concrete degradation.
9. The potential interaction of Fe^{2+} from anaerobic corrosion of steel with cement and concrete is a ‘new’ topic, and as such, relevant research has not been reported by other waste management agencies. Nevertheless, this issue could potentially have a large impact upon concrete degradation processes and near-field pH so that SSM needs to ask SKB what it plans to do about the issue in its future R&D programme.
10. It is not clear in any of the relevant reports the precise state of the bentonite as emplaced in the Silo. Has it been emplaced in compacted form? If so, at what density? Or is the bentonite in powered/pelleted form? Some clarification is required. In addition, SSM should ask SKB for clarification of the issue of how bentonite might have resaturated with cement pore fluids in the Silo.

APPENDIX 3

Suggested review topics for SSM

1. SSM should carry out its own study of potential controls of water-rock reaction at the SFR site using thermodynamic activity diagrams with groundwater data made available by SKB. This study should attempt to link observations of groundwater chemistry and mineralogical evidence from drillcores to produce a more holistic view of water-rock reaction at the SFR site.
2. SSM should re-evaluate the potential for up-coning of saline groundwater from depth to confirm SKB's conclusions on this issue.
3. The report by Vidstrand et al. (Vidstrand et al., 2006) on the exclusion of the effects of salt exclusion during periglacial conditions should be reviewed to assess the validity of SKB's conclusion that any occurrence of salt exclusion in the past would have been flushed from the rock-groundwater system.
4. The effects of saline groundwater on concrete degradation should be modelled to assess rates of degradation and potential changes to pH.

2016:08

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.

The Swedish Radiation Safety Authority works proactively and preventively to protect people and the environment from the harmful effects of radiation, now and in the future. The Authority issues regulations and supervises compliance, while also supporting research, providing training and information, and issuing advice. Often, activities involving radiation require licences issued by the Authority. The Swedish Radiation Safety Authority maintains emergency preparedness around the clock with the aim of limiting the aftermath of radiation accidents and the unintentional spreading of radioactive substances. The Authority participates in international co-operation in order to promote radiation safety and finances projects aiming to raise the level of radiation safety in certain Eastern European countries.

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