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Swedish Radiation Safety Authority

2017:33

SSM's external experts' review of SKB's safety assessment SR-PSU – dose assessment, K_d-values, and safety analysis methodology

Main review phase

Report number: 2017:33 **ISSN:** 2000-0456
Available at www.stralsakerhetsmyndigheten.se

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 during the main review phase. 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 an in depth assessment of the specific issues defined for the different disciplines. In 2017 SSM held a workshop on interdisciplinary aspects of the review of the safety analysis SR-PSU, which is also reported in this volume.

Project information

Contact person SSM: Georg Lindgren

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

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This report concerns a study which has been conducted for the Swedish Radiation Safety Authority, SSM. The conclusions and viewpoints presented in the report are those of the author/authors and do not necessarily coincide with those of the SSM.

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Review of dose assessment landscape models – main review phase

Activity number: 3030014-1006
Registration number: SSM 2015-1020
Contact person at SSM: Shulan Xu

Abstract

SKB has submitted an application to extend the SFR repository for low- and intermediate-level radioactive waste at Forsmark. Following a preliminary review carried out to identify themes for a more in depth review, this report presents the outcome of the main review of the material relating to the dose assessment modelling carried out by SKB in the context of the release and distribution of radionuclides in the future landscape around the Forsmark site.

The aim of the review has been to determine the suitability of the SR-PSU documentation, specifically in respect of how key aspects of the biosphere system are identified and their interpretation justified in the definition of the dose assessment modelling. The review has therefore addressed technical issues of the interpretation of site descriptive material as well as how this material is used to define the landscape dose model as applied in the SR-PSU assessment. Attention is also given to possible alternative interpretations.

As far as can be determined by this review of the SR-PSU documentation and supplementary material from SKB's response to the RFIs (requests for further information) formulated during the initial review, there are no obvious omissions from the SR-PSU assessment. The doses calculated are credible and the methodology is broadly appropriate. The only misgivings come from the decreasing completeness of the documentation as the reports move from the well documented site descriptive material to the details of the dose assessment modelling and how this is integrated into the overall assessment. There are a number of instances where supplementary analyses should have been carried out to support the main findings. Alternative conceptual models and implementation would help build confidence in the SR-PSU results. Some of these issues have been recognised by SKB and are expected to be addressed future iterations of SKB’s assessment modelling for both the low and intermediate level repository and the planned spent fuel repository at Forsmark.

Contents

1. Overview of SR-PSU Main Phase Review

1.1. Background

The Swedish Nuclear Fuel and Waste Management Co., SKB, submitted an application for an extension to the Forsmark low and intermediate level waste disposal facility (the SR-PSU Assessment: SKB, 2014a) to the Swedish Radiation Safety Authority (SSM) at the end of 2014. On behalf of SSM, Dr Richard Kłos (Aleksandria Sciences Ltd, UK), Professor Anders Wörman (KTH Stockholm, Sweden) and Professor George Shaw (University of Nottingham, UK) carried out an initial review of the published material in SR-PSU during 2015. This report details the results of the main phase review carried out during 2016 by Kłos & Wörman. The main phase review by Prof. Shaw is reported elsewhere (Walke *et al*., 2017).

SR-PSU is a comprehensive and highly detailed assessment of the potential for the release, transport and any subsequent exposure to radionuclides disposed in the SFR1 for low and intermediate level radioactive waste and proposed SFR3 for radioactive decommissioning waste. The time period over which detailed assessment is carried out is 100 kyear during which time there is rapid initial evolution of site conditions from coastal to terrestrial ecosystems. In the longer term, beyond 10 kyear AP (after present) it is expected (as a result of detailed modelling of landscape evolution in the project) that the landscape will approach a state of dynamic equilibrium with relatively little further significant change.

There were a number of requests for further information (RFIs) that arose from the initial review. A meeting between SSM, SKB and the review team in April 2016 resolved a number of the issues but a number remained for deeper investigation and these were forwarded to SKB with the requested material being provided in the autumn of the same year.

This main phase review therefore includes further consideration of the material in the published reports included in the initial phase review (SSM, 2016a) but also includes a more detailed review using data from SKB's response to the RFI. Appendix 1 gives further information concerning the Request for further information with SKB's response.

The Biosphere FEP (Features, Events and Processes) report (SKB, 2014b) was also reviewed here. This was not part of the initial phase review, only becoming available shortly before the main phase review commenced.

1.2. Approach to the main phase review

In the SR-PSU documentation SKB provide a complete and plausible narrative for the evolution of the repository structures, radioactive waste containment, radionuclide migration and distribution in the surface environment together with a representation of the exposure pathways by which the future population (human and non-human) may receive doses from environmental accumulations of any radionuclides released from the repository.

The issue in this detailed review, is the appropriateness and the completeness of the description and analysis in the SR-PSU documentation. The aim of this main review

phase is to address options for alternative interpretations and to assess the extent to which the alternative conceptualisation might influence the results obtained and the conclusions drawn in the SR-PSU documentation.

Essentially there are three main themes to the review.

- The treatment of landscape evolution in the dose assessment modelling
- The implementation and interpretation of key FEPs in the dose assessment model
- Probabilistic modelling in SR-PSU

These are addressed in each of Sections 2 to 4. Section 5 provides a discussion of the results of the review. Conclusions are given in Section 6.

2. Landscape dose modelling

2.1. Release locations – the key landscape objects

The biosphere synthesis document (SKB, 2014c) describes the biosphere for the dose assessment at a high level. The description of the evolution of the landscape encompasses a large area (as in SR-Site; SKB, 2011). This is to be expected but, in contrast to the SR-Site assessment, the details on page 98 of the biosphere synthesis report (temperate conditions) and page 100 (periglacial conditions) show that the objects in the biosphere that are likely to be affected by any releases from the SFR repository are restricted to small areas within two to three km of the repository.

A new digital elevation model (DEM) of the current topographic surface (regolith depth model - RDM) has been produced for SR-PSU (Strömgren & Brydsten, 2013). Both current land surface and bathymetry have been remeasured to produce the *reference DEM* for the assessment, superseding the DEM used in earlier assessments (SKB, 2008; SKB, 2011). The reference topographic surface in the new DEM is then both "aged" and "youthed" using the erosion and deposition models in the Regolith-Lake Development Model (RLDM) described by Brydsten & Strömgren (2013) to give deterministic models in each of the different climate sequences[1] for the evolution of regolith and lakes systems from 8500 BCE to 40 000 CE at 500 year intervals over the entire landscape model area. Figure 1 shows the full extent of the RLDM.

The calculated regolith thickness maps that have been provided in response to the RFIs have been used to visualise the relevant parts of the system at key times. Figure 2 shows the releases at 9000 CE in the 9000 CE landscape model. The area is as indicated in Figure 1. The main area affected lies close to the location of the repository (biosphere objects receiving releases identified by SKB are outlined in dark blue). Using the data in the dataset provided by SKB in response to the initial phase RFI's the thickness of the regolith in the vicinity of the releases is also available, as indicated by the colour-coded regolith thickness contours.

Release locations have been determined by particle tracking with releases from repository depth (from the material in Odén *et al*., 2013). The end point of the calculation is the location of the particles' release at the top of the bedrock. As mapped in Figure 2, the release locations are shown as *release point density* as calculated by the mapping software. The advantage of this is that the spatial distribution in the landscape is shown and, more importantly, the locations where the highest concentration of releases is more clearly seen than if the points themselves are plotted.

The subsequent fate of the releases is the domain of the biosphere and it is one of the main themes in the radionuclide transport modelling in the dose assessment model. The release points calculated by Odén *et al*. (2013) link parts of the repository from which radionuclides might be released to the positions at the bedrock-regolith interface where they enter the biosphere system. The spatial distribution of the release locations from the repository structure therefore means that simultaneous release to multiple release points is likely and that the distribution and concentration of release points carries more practical information for SFR than did the release point distribution in SR-Site, where each location was associated with the failure of a single spent-fuel canister. From the SR-PSU documentation it is not clear if the spatially extended release footprint is important to the estimation of radiological impact.

[1] The alternate climate sequences are: Global warming case, early periglacial case and Weichselian glacial cycle case.

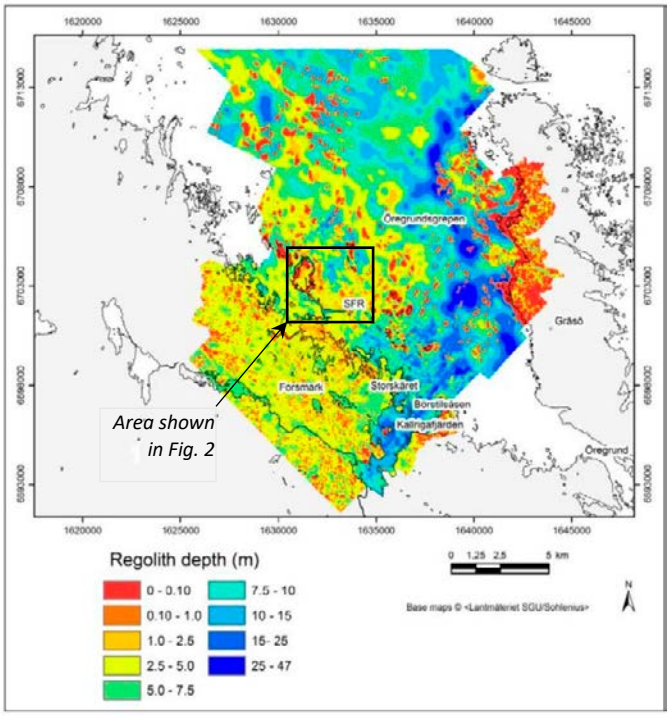


Figure 1. Total modelled regolith depth. Taken from Fig. 5-1 on page 38 of Strömgren & Brydsten, 2013.This figure shows the extent of the area covered by the regolith and lake development model reported by Brydsten & Strömgren (2013).

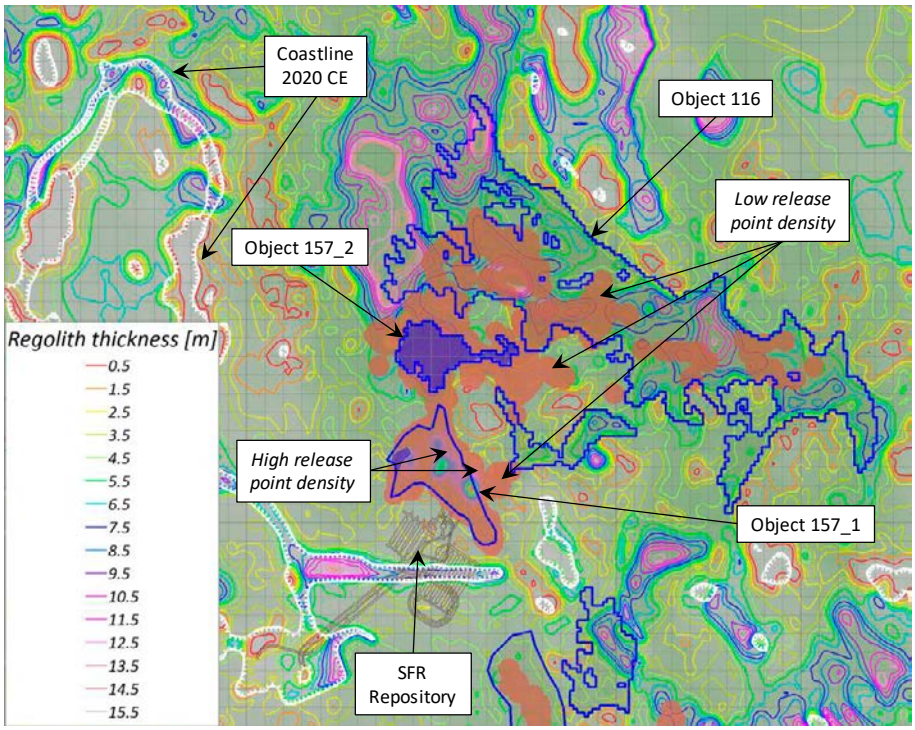


Figure 2. Map of the release area for temperate conditions based on material provided by SKB in the response to the RFI. Regolith thickness contours and density of release locations are indicated in the context of the topography at 9000 CE See also Figures 3 and 4.

The topography of the surface is related to the definition of landscape objects. Because the regolith hydrology of the Forsmark region is delineated mainly by discrete basins largely defined by the bedrock topography, the areas of the landscape objects do not change in time but their vertical characteristics do, as sediments accumulate and the upper layers, particularly the peat, mature. The lakes infill over time.

The landscape at 9000 CE is significant since, by this time, the hydrology is close to its long-term steady-state condition with the coastline (a bay of the future Baltic) in the deeper parts of the topography some 5 km to the east with a SE-NW axis. Thereafter further landrise results in the formation of relatively deep lakes to the north-east around 8 km away. Beyond 9000 CE then the major changes at the release sites will be as a result of the maturation of the vegetation or as a results of human perturbations to natural condition.

2.2. Biosphere objects: Evolution and interpretation

Two main documents are used to determine how the landscape evolves over the course of the assessment, one on the RLDM (Brydsten & Strömgren, 2013) and one on the hydrology (Werner *et al*., 2013). The interaction between these areas of knowledge is important. The base digital elevation model (the DEM; Strömgren and Brydsten, 2013) is the starting point, expressing the known present-day topography.

The DEM data provided by SKB illustrates the potential uncertainty in the representation of the topography of the landscape around the release areas, particularly in respect of how the key basin Object 157 is interpreted. Alternative interpretations, based on the SKB maps are shown in Figure 3 (subcatchments and implicit surface drainage system using the reference DEM) and Figure 4 (subcatchments and drainage for the 9000 CE DEM). The two maps show the SKB-defined objects and the density of release points.

Of interest are the two "lakes" or "ponds" in the base DEM. The large of the two (shaded blue) is in Object 157_1, downstream of the release area. The smaller is in 157_2, though not coincident with the highest release point density. These are identified by closed contour depressions in the base DEM. As such it is to be expected that they will be the locations of sediment accumulation during the transition millennia from the present day marine to future terrestrial environments. They therefore define the maximum extent of surface water features in the future landscape. The 157_1 object has an area of 6.7×10^4 m^2 and maximum depth of 2 m. The 157_2 "pond" is much smaller (7.3×10^3 m^2) and maximum implied depth of only 20 cm.

On this analysis it seems plausible to rule out standing water objects in Object 157_2. Indeed, the RLDM maps of the objects show that the 157_2 pond is rapidly infilled and never forms a "pond". Similarly by 5000 CE (shortly after emergence of the object) the 157_1 "lake" has area 5×10^4 m^2 with maximum depth of around still 2 m. The reduction of area is around the perimeter with reed beds making up the majority of the shallow areas. By 9000 CE the object (which corresponds closely to the outline determined by SKB's analysis) is likely to be a wetland mire.

The area of the 157_1 "lake" is of reasonable size but the lake is not large enough to form a significant proportion of the diet from fish *in its natural state.* The emphasis is used to stress the possibility that there may be human induced perturbations to this natural state that should be addressed in the assessment. It is unlikely that, say, fish farming would be undertaken in either of the locations. The issue for the assessment is the potential for dose if it were to be.

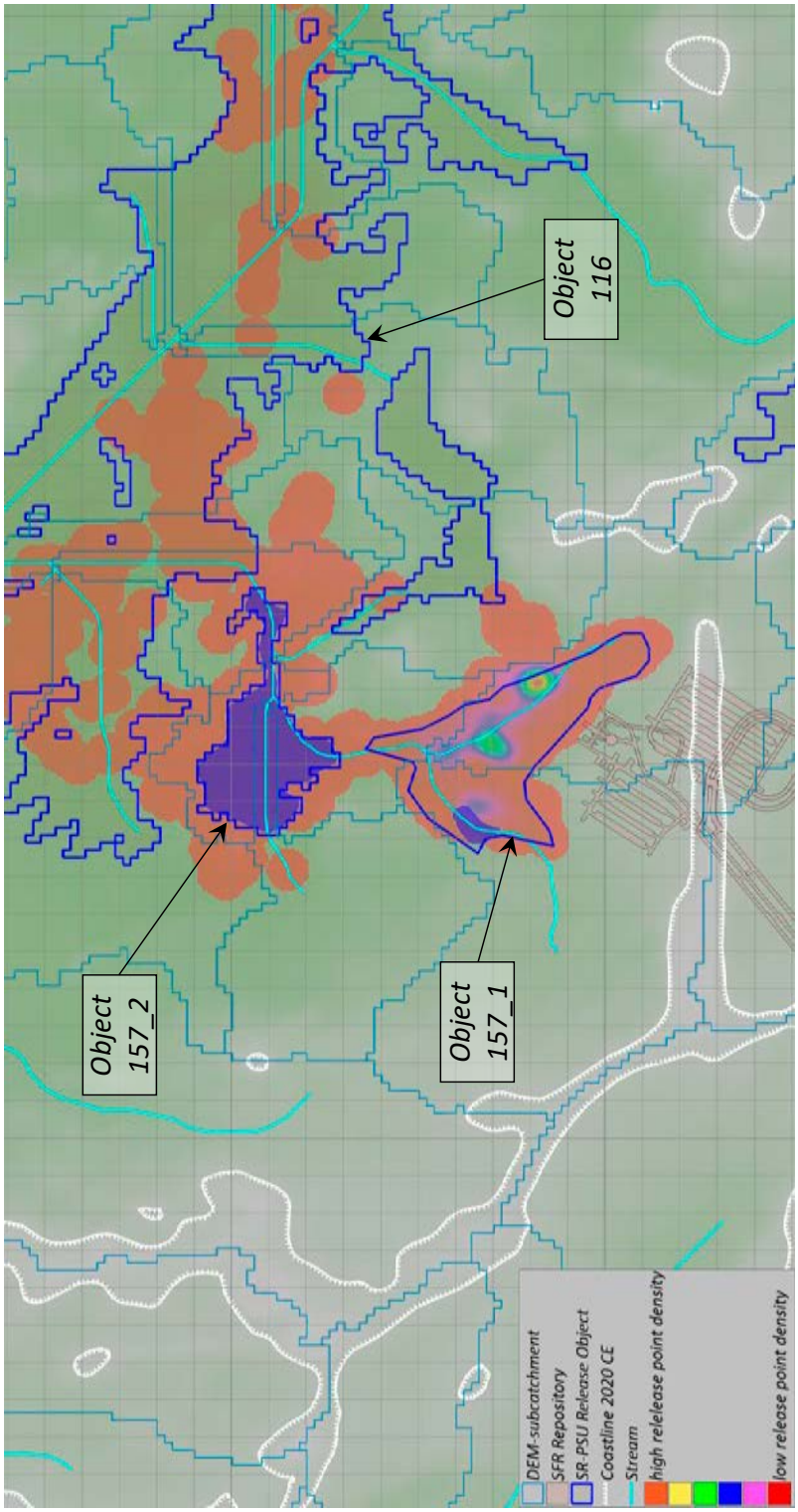


Figure 3. Subcatchment areas and streams interpreted by Global Mapper 17 GIS mapping software (www.globalmapper.com) using reference DEM from Strömgren & Brydsten (2013). Closed basins shown by blue areas. Colour scale indicates release point density. The infilled blue areas denote depressions in the reference DEM where water bodies could form. Streams are the locations of preferential flow derived by Global Mapper based on the topography.

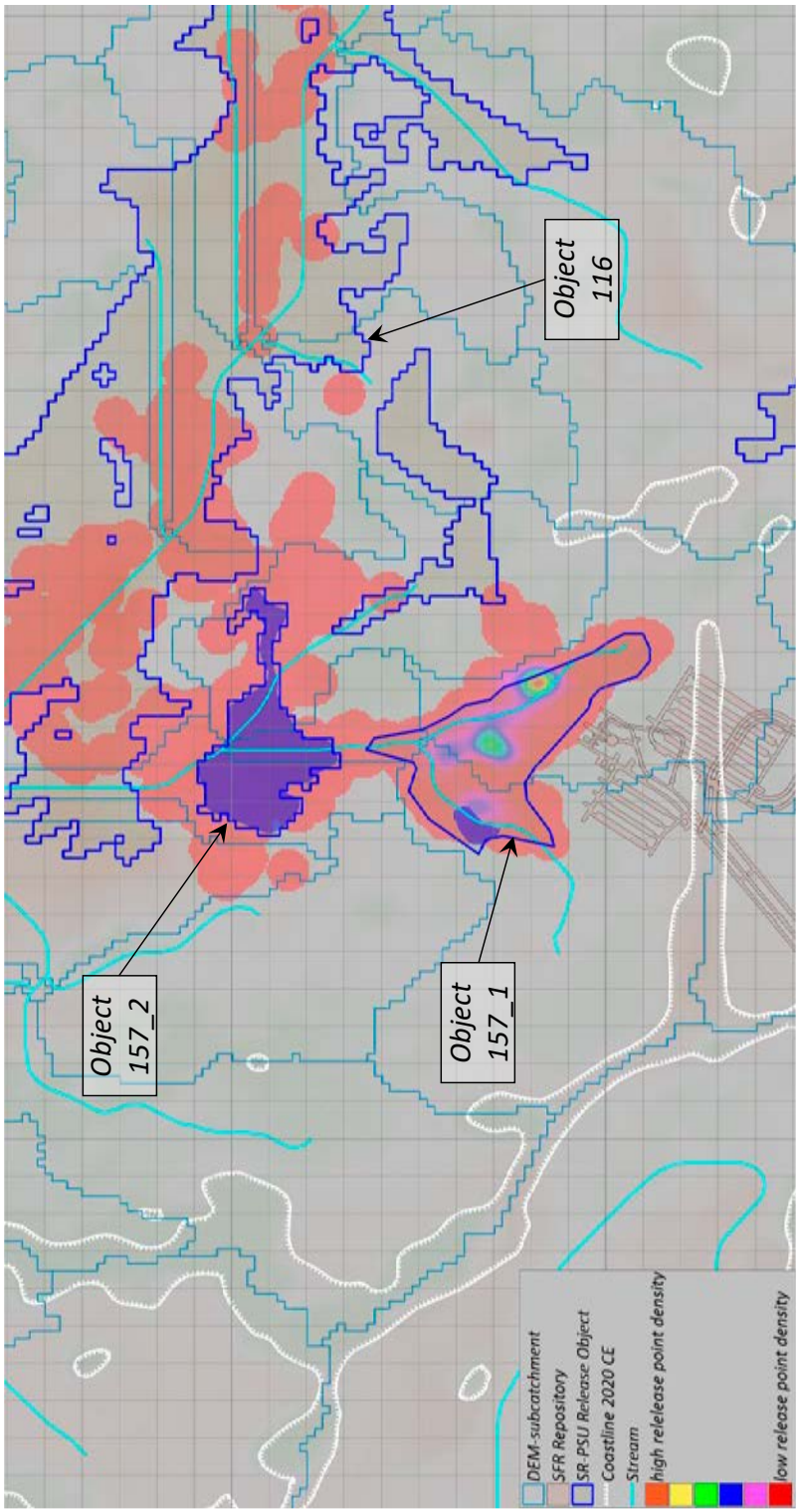


Figure 4. Subcatchment areas and streams interpreted by Global Mapper 17 GIS mapping software (www.globalmapper.com) for the topography of evolved landscape at 9000 CE produced by the RLDM of Brydsten & Strömgren (2013). The closed basins shown by blue areas in Figure 3 are also displayed here. These would be infilled in the 9000 CE landscape. Locations of potential water bodies in the reference DEM are shown for illustrative purposes. The subcatchment boundaries are similar to those for the reference DEM in Figure 3, with differences arising from the changes to the accumulated regolith. This also produces minor changes to the location of surface water streams.

The other type of surface water feature is, of course, the stream network. The maps shown here illustrate that the sub-catchments in the surface system are amenable to assessment using GIS tools. For the reference DEM map and the topography calculated for 9000 CE in the RLDM the estimated catchment areas are outlined in pale blue. The similarity between the two topographies (Figure 3 and Figure 4) illustrates that the RLDM introduces only small perturbations to the reference DEM. Nevertheless there are clear differences in the interpreted surface drainage system (stream network – shown in cyan). However, this is to be expected as the differences in the stream networks are a consequence of the relatively flat topography.

Catchments in object 157_2 remain largely constant with the evolution of the upper regolith. In 157_1, however, there are changes to the subcatchment areas and to the positions of the implied surface drainage streams. This reflects the flattening of the regolith in these areas with the growth of sediment in the lake bed. The flow systems become less well defined and while there might be preferential flow paths in these wetland areas a precise picture of the stream network is not a realistic expectation. The visualisation in Figures 3 and 4 should therefore not be treated as a prediction of the future but in terms of guidance.

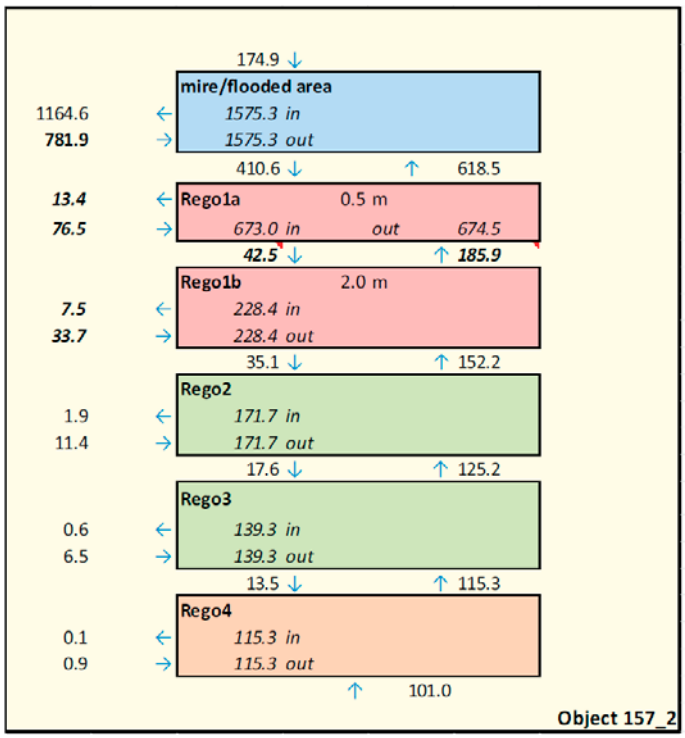
It may be expected, on the basis of the RLDM, that the hydrology of the 157 lake and wetland area will change during the period from the emergence of the top of the sloped area that constitutes Object 157_2 (from around 3000 CE) to total emergence of the object (at its northern extent at around 4500 CE). An important consideration is how the groundwater flow vectors in the objects are determined. The catchment maps in Figures 3 and 4 can be used to determine the water flows in each of the subcatchments, being determined as the product of subcatchment area and runoff (precipitation – actual evapotranspiration).

The identification of the basins and their subcatchments provides a useful visualisation tool for the construction of the dose assessment model. The chosen method of SKB – to use MIKE-SHE to determine the groundwater flow system in the objects is thereby supported with the advantage that the topographically derived stream network (i.e. slope-following paths in the landscape) gives a clear visualisation of the landscape at future times.

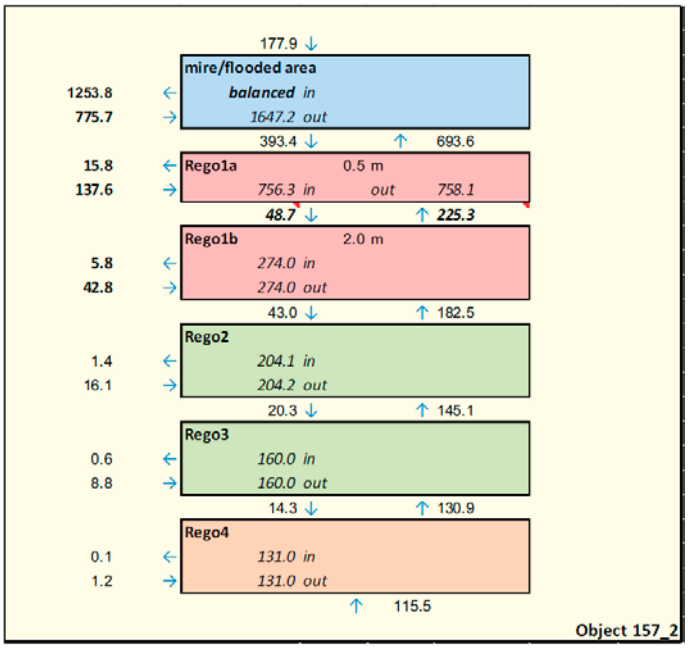
There is a heavy reliance on the working of MIKE-SHE in the SKB approach to modelling. One issue raised in the initial phase review concerned the derivation of water fluxes into the biosphere objects: *Derivation of object water fluxes from MIKE-SHE modelling. Comparing the details … SKB should illustrate how the SKB results for the landscape … are converted into the detailed inter-compartment numerical values quoted.* (SSM, 2016b, page 5).

The response from SKB was that the "details" are as set out in Section 7.2 of Werner *et al*. (2014). In fact this section of Werner *et al*. sets out the *outline* of the procedure rather than giving *details*. However, the procedure, having identified the object's boundaries, is consistent with and produces results that are similar to what might be expected using the topographic information to define the broad hydrological connections for the release objects in the landscape of the topographic basins.

Once the boundaries of the objects are determined there are routines within MIKE-SHE that calculate mass balance and output the numerical results interpreted in the SR-PSU documentation as illustrated in Figure 5 for Object 157_2 at 5000 and 11000 CE. These are the raw data that are transmitted to the radionuclide transport model (with a compilation of sorts in Grolander, 2013). However, the mathematical description of the FEPs is given in Saetre *et al*. (2013a) and it is left to the biosphere synthesis document (SKB, 2014b) to attempt to link all this information – FEP expressions and numerical data – together.



(a) at 5000 CE (Figure A1-42) of Werner *et al*. (2014)



(b) at 11000 CE (Figure A1-49) of Werner *et al*. (2014)

Figure 5. Water balance for Object 157_2 at two times (a) 5000 CE and (b) 11000 CE. The differences in results come from changes in parameters in MIKE-SHE, such as vegetation cover. Fluxes are quoted as mm year^{-1} normalised to the area of the object. Interpretation of the different regolith layers is discussed in the text.

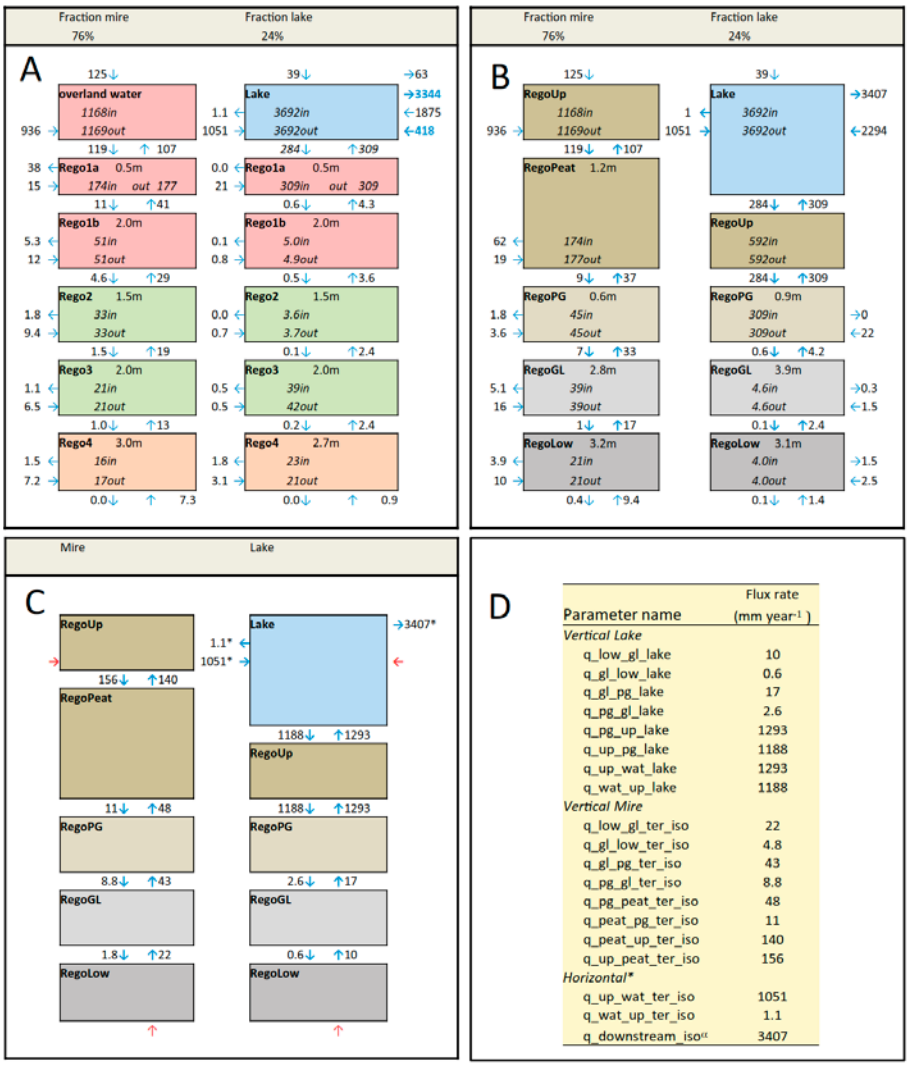


Figure 7-19. *Calculation of water fluxes (mm/y) across regolith layer boundaries. A) MIKE SHE-calculated water-balance components for biosphere object 157_1 at 5000 AD. B) Estimated across-layer fluxes. C) Fluxes delivered to the radionuclide transport modelling, scaled according to relative sizes of lake and mire areas. Red arrows represent potential release pathways for radionuclides (surface water from object 157_2 or groundwater discharge from the rock). D) Parameter names and associated inter-compartment water fluxes delivered to the radionuclide transport modelling (cf Table 7-19). used in the radionuclide model. *Horizontal surface-water fluxes retain original units (fluxes are scaled per unit object area).*

Figure 6. Illustration of the obscurity of the SR-PSU documentation. Figure 7-19 from the surface hydrology report R-13-19 (Werner *et al.*, 2014). Stages in the interpretation of MIKE-SHE output for the radionuclide transport model for Object 157_1 at 5000 CE. Attention is drawn to the asterisk in panel D, referring to the description of the horizontal fluxes of water.

If the preceding paragraph seems somewhat convoluted and obscure this serves to illustrate the parallel difficulties in reviewing the documentation when set out in this way. Figure 7-19 of Werner *et al*. (2014) exemplifies the difficulties. It is reproduced, in full, here as Figure 6. The procedure is **not** criticised for being incorrect or inappropriate. Rather, it is that the procedure from panel A to panel D is insufficiently clear. Not all of the numerical values in A are readily traceable to B with renormalisation being carried out between A and C. The most important feature is the absence of lateral fluxes in B, with the mire and lake systems being treated independently.

In Panel C the numerical flux values are identified and their corresponding parameters names are given in panel D. However, the comment in panel D that *Horizontal surface-water fluxes retain original units (fluxes are scaled per unit object area)* is entirely unhelpful. This is not the "detailed" explanation sought, it is an overview. The nearest the documentation gives to a discussion of the actual rationale is found on page 32 of Saetre *et al*. (2013a):

> *The horizontal transport of water in sub-surface layers, (i.e. in consolidated peat, lacustrine sediments, glacial clay and till), is expected to be small compared with vertical fluxes between regolith layers (occurring over distances that are orders of magnitude shorter) in future lakes and wetlands in Forsmark (Werner et al. 2014).* ***For simplicity, horizontal transport below the top regolith layer between ecosystems or between biosphere objects is not explicitly represented in the radionuclide transport model***. [Emphasis added].

The procedure for determining fluxes therefore appears to be: 1) Identify object boundaries, 2) Setup MIKE-SHE with the objects boundaries **and** selected vertical discretisation, invoke water balance output and 3) Reinterpret fluxes for radionuclide transport model (with restrictions on horizontal fluxes *for simplicity*). The implications of this simplification are not further addressed. It is not clear at which stage of model development this decision was made.

There are some important modelling choices here:

- the vertical resolution of the MIKE-SHE model – chosen to match the conceptualisation of the radionuclide transport model, rather than the stratigraphy of the object,
- simplification of lateral fluxes in the mire-lake interaction,
- The identification of some "inputs" that include fluxes of radionuclides from other parts of the landscape and geosphere.

The vertical structure of the radionuclide transport model in the dose assessment model is determined to comprise the upper layer (*RegoUp* – unsaturated soil layer or top layer of aquatic sediment) and layers for saturated peat, post glacial clay and glacial clay (respectively *RegoPeat*, *RegoPG*, *RegoGL*). These lie atop the lower regolith Till layer (*RegoLow*). The properties of the MIKE-SHE discretisation are chosen – and to some extent interpreted – to match this division so that the results from the MIKE-SHE calculations are more readily translatable into data for the transport calculations.

The biosphere FEP report (SKB, 2014b) investigates the possible implications for alternative discretisations in MIKE-SHE, with emphasis on a vertical resolution that more closely matches the hydraulic character of the different regolith media to compartments in the model. In the sensitivity analyses in the biosphere FEP report (2014b) the different MIKE-SHE representations of Lake Stocksjön take as their basis a more exact implementation of the stratigraphy of the regolith in the Stocksjön basin. In the standard representation there are two MIKE-SHE layers for the entire regolith (regolith total thickness around 5 – 6 m). One sensitivity study case –

7CalcL_1 – models each of the seven geological layers by a dedicated layer in the MIKE-SHE calculation. Results are reported to show that: *for the cases with an increased number of calculation layers in the regolith, the upward flow is higher than for the cases with only two calculation layers.* Furthermore the hydraulic properties of the different layers are such that, if the full set of layers is included, the horizontal flow is increased. Rather than entering the surface layers vertically above the source of the groundwater input from the bedrock, the flow would reach the surface somewhere "downstream". For the analysis of Lake Stocksjön this remains something of a curiosity in the modelling. For Object 157_2 the implications are potentially more significant in terms of transport of radionuclides to, and accumulation in, the surface layers, potentially of Object 157_1.

The results of this analysis are, however, not carried forward to the sensitivity studies in support of the dose assessment modelling, possibly as a consequence of the late finalisation of the biosphere FEP report (SKB, 2014b), which was released for review just prior to the start of the main phase review. It is not clear if this delay meant that consideration of the results from the MIKE-SHE sensitivity study were therefore unavailable for the SR-PSU dose assessment studies.

The processed interpretation of the hydrology of Object 157_1 assumes that water fluxes between objects are mediated at the top layer of the compartment structures – RegoUp or surface water compartments. In Figure 5, water fluxes calculated by MIKE-SHE for Object 157_2 (which has no lake stage) imply that some flow in the sub-surface regolith layers would be possible. However, all of the water flows are subsumed into the upper layer in the radionuclide transport model[2]. Depending on the disposition of ^{14}C in the soil profile this could reduce the outflow of ^{14}C from 157_2 (where it accumulates) into the mire/lake system of 157_1. The conclusion in the biosphere synthesis report that ^{14}C is predominantly lost from the 157_2 soils by degassing before entering object 157_1 may be an artefact of the chosen radionuclide transport model structure.

Overall then, the relative unimportance of ^{14}C in SR-PSU is not robustly demonstrated in the sensitivity analyses reported in the SR-PSU documentation. For other radionuclides important in the assessment the assumptions concerning water fluxes would tend to be more conservative in that the radionuclides would be retained in the deeper regolith layers of the release object at 157_2.

The Lake Stocksjön sensitivity analysis (SKB, 2014b) implies that a sensitivity analysis for Object 157_2 with a more precise description of the stratigraphy of the regolith in the object would have an influence on the distribution of radionuclides in the upper layers of the regolith around the 157_2 release locations. It is not satisfactorily verified that the sensitivity analysis of lateral discretisation captures the impact of the uncertainty in the vertical discretisation.

The sensitivity analyses carried out in respect of the object delineation in 157_2 are practical but there is more to investigate. From the Lake Stocksjön analysis it seems that there is potential for a downslope accumulation at the lower elevation of the object. This corresponds to the "agricultural area" defined in one of the alternative delineation cases but it is not clear that the assumptions in the 157_2 sensitivity study (of doses) are equivalent to the case that would arise if a more complete model of

[2] The water flux from the "mire/flooded area" of 157_2 in Figure 6 suggests that there is a significant flow of water from the model layer above *Rego1a*. This lends credibility to the topographic interpretation of the drainage streams as shown in Figures 3 and 4. The illustrative potential of working with the topographic maps is thereby further enhanced. Saetre & Ekström (2016) have analysed the situation as stream flow and concluded that there is little impact on calculated dose.

157_2 and its structure were implemented in the biosphere radionuclide transport model. A lot depends on the accuracy and reliability of the landscape development model.

Further safety analyses on Object 157 as a whole, with an alternative conceptualisation would enhance confidence in the dose modelling in Object 157_2 and the possibility of ^{14}C reaching the lake in 157_1 in significant quantities would be addressed. Overall the assessment would benefit from a more complete narrative of the fate of radionuclides entering object 157_2 at the base of the till layer.

2.3. Taliks in landscape dose modelling

The timescale of dose modelling in the SR-PSU assessment is 100 kyear. There are three main climate scenarios included in the assessment to account for changes over this period (SKB, 2014g). Two are variants on the present day climate ("Global Warming" and "Enhanced Global Warming") with one that assumes the possibility of an early periglacial episode of limited duration (a few kyear) corresponding to a solar insolation minimum at around 17 kyear after present (19000 CE). Periglacial conditions would not return until after 50 kyear AP (after present) when the climate sequence follows that in the base scenario (the "global warming scenario"). Only in the extended global warming scenario is there no periglacial state.

In the SR-Site assessment a considerable amount of preparation was carried out to develop techniques for describing periglacial conditions (Bosson *et al*., 2010) but only in SR-PSU is this material carried over in to the landscape dose modelling since the timescale for dose assessment modelling in SR-Site was only up to 10 kyear AP compared to 100 kyear AP in SR-PSU. The methods have been updated somewhat for SR-PSU (Bosson *et al*., 2013). Permafrost conditions have a clear impact on the state of the hydrology of the regolith. Contact between radionuclide bearing groundwater in the bedrock and the surface is therefore expected to be via open taliks. Groundwater flows are, as with the temperate case, modelled using MIKE-SHE.

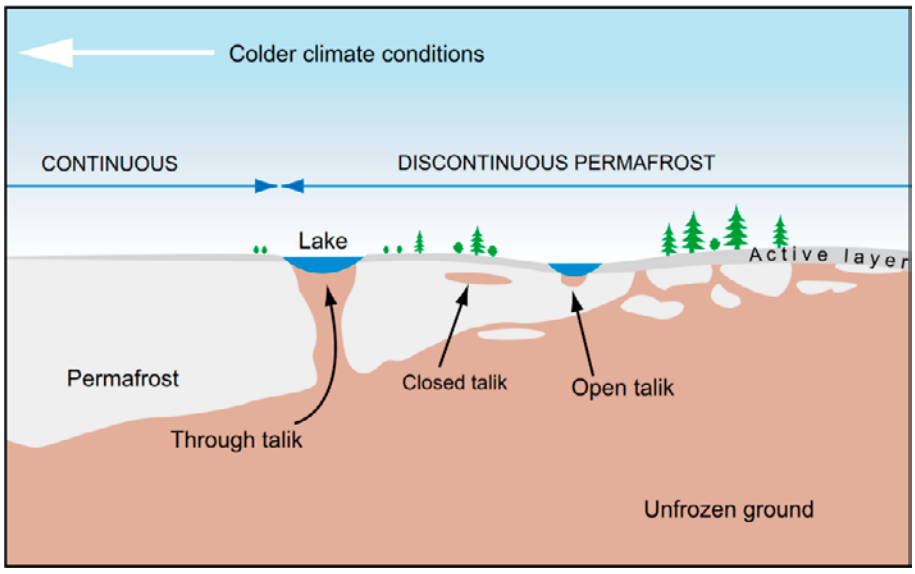


Figure 7. Sketch of deep-surface hydrology in permafrost conditions. Taken from Bosson *et al.* (2010) and used as Figure 4-8 in the biosphere synthesis report for SR-PSU (SKB, 2014c).

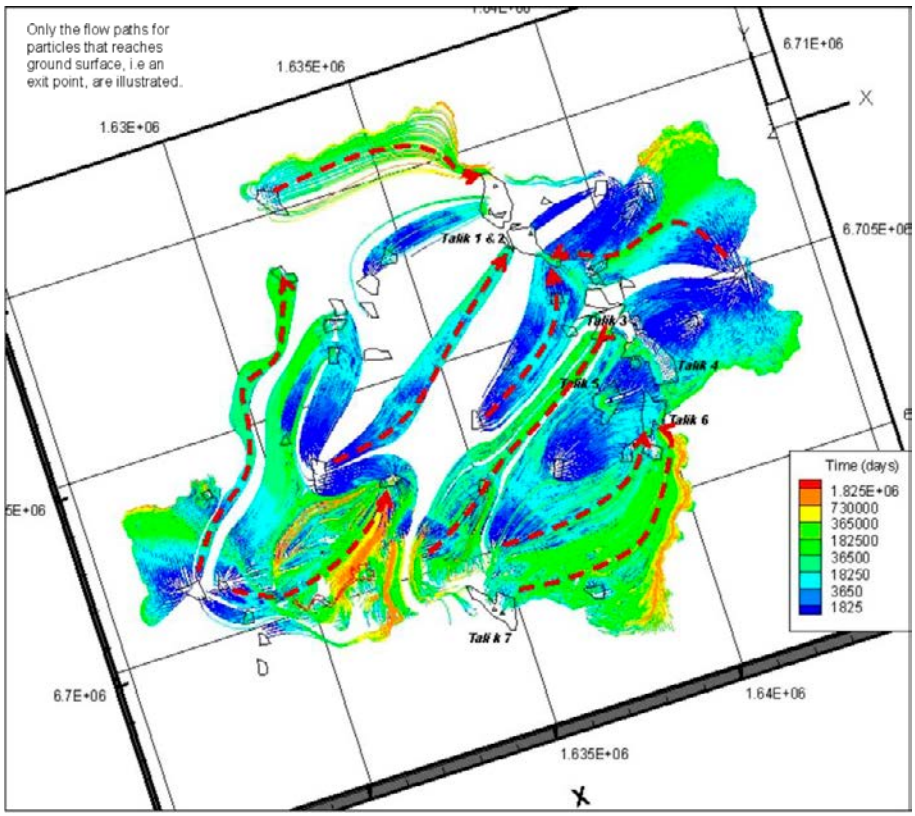


Figure 8. Illustration of flow paths of particles released below the permafrost during the active period (case 100mPf_active_belowpf). The illustration is a horizontal view from above, and the colour along each flow path shows the accumulated particle travel time (in days).

The MIKE SHE regional model is used to calculate water fluxes that are used to parameterize ECOLEGO rate coefficients. According to R-13-19 the model domain has an area of around180 km^2 and a vertical extent down to –634 m elevation. The model boundaries follow water divides according to the DEM at which no flux boundaries are assumed. The top boundary conditions are based on the precipitation (P) and the potential evapotranspiration (PET). The P and PET are assumed to be uniformly distributed over the area and are given as time series. In the MIKE SHE model describing future conditions in the Forsmark catchment, lateral inflows via streams exist and occur in five discrete points (Bosson *et al*, 2013). The implication of these boundary conditions combined with the fact that permafrost is represented simply by changing the hydraulic conductivity imply that there is a certain (though probably very small) flow through the permafrost layer. On top of the permafrost layer there is a 1 m thick "active layer" through which the surface hydrological processes are maintained in the MIKE SHE model (Figure 4-8, TR-14-06, reproduced as Figure 7). The paper by Bosson *et al*. (2013) further describes

> *A number of through taliks, unfrozen areas in the permafrost …, are further simulated under permafrost conditions as objects (model volumes) with the same hydraulic properties as under temperate climate conditions.*
>
> *Under modelled permafrost conditions, through taliks are therefore only present under lakes, while the too small streams and lakes are still surface-water bodies under such conditions.*

Figure 6-65 in Bosson *et al*. (2010) (as Figure 8) shows recharge taliks connects the groundwater flow to discharge taliks, which are the areas that dominate the exchange between groundwater and surface water, except for the exchange with the sea and the very low flow through the permafrost layer.

Werner *et al*. (2013) states:

> *As described previously, fluxes obtained from the water-balance tool in MIKE SHE are mapped to relevant compartments of the radionuclide transport model …. Upward and downward vertical fluxes across regolith layer boundaries are estimated under the assumption that fluxes across calculation layer boundaries, at which MIKE SHE calculates fluxes, change linearly with depth in each MIKE SHE calculation layer. Hence, for each biosphere object upward and downward fluxes are calculated to obtain corresponding net fluxes at each regolith-layer boundary at the times 3000, 5000 and 11,000 AD.*

The calculated water fluxes are found in Appendix 1 in Werner *et al*. (2013 - Figures A1-64 and A1-65, Figure 9 here). All fluxes are "mapped to relevant compartments" of the radionuclide transport model that is used to calculate doses to humans. In addition there is an attempt described in Werner *et al*. to study the influence of object delineations for biosphere object 157_2. This object was divided into subareas for which water balances were extracted and delivered to the radionuclide-transport model. However a similar delineation was not done for the permafrost cases and it is uncertain to what extent this information was used to parameterize the radionuclide transport model.

In respect of the translation to Ecolego modelling Werner *et al*. go on to say

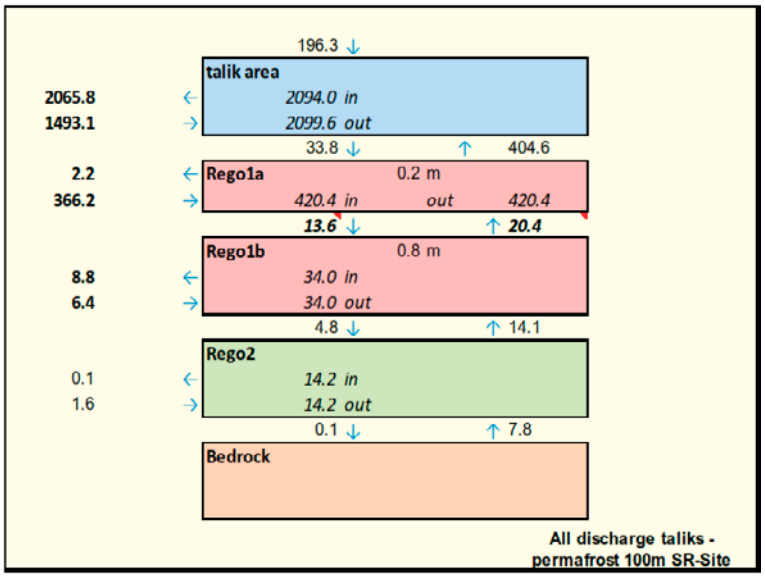
> *Upward and downward vertical fluxes across regolith layer boundaries are estimated under the assumption that fluxes across calculation layer boundaries, at which MIKE SHE calculates fluxes, change linearly with depth in each MIKE SHE calculation layer. Hence, for each biosphere object upward and downward fluxes are calculated to obtain corresponding net fluxes at each regolith-layer boundary at the times 3000, 5000 and 11,000 AD.*

Further, Appendix 1 in Werner *et al*. summarises the water balances, which appears to be relevantly represented in the figures A1-1 to A1-6. Also figures A1-31 to A1-66 presents water balance values (Figure 9 here). A main finding is the following:

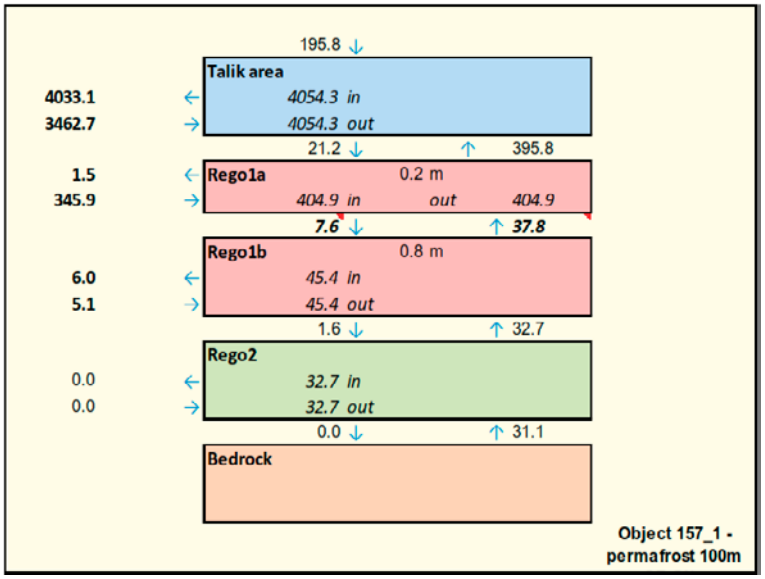
> *In the permafrost case (Table 7-16)* [as Table 1 here]*, the net vertical groundwater flux from rock to regolith in biosphere object 157_1 is three times the corresponding flux at 11,000 AD for a temperate climate …. Moreover, the flux from regolith to the surface is more than ten times larger in the permafrost case.*

This should imply a faster exchange in the regolith of object 157_1 during permafrost conditions, although there are several questions that can be raised regarding this finding.

There are a number of issues arising from the inclusion of taliks and associated hydrology into the model. Focussing – where contaminated water fluxes from the bedrock enter the biosphere release object over an area less that the dimensions of the entire object – is known to be important from the SR-Site modelling. It is likely that similar processes are relevant to talik hydrology. In other respects, however, with the modelling in MIKE-SHE, taliks are simply interpreted as modified lakes in the periglacial MIKE-SHE landscape.



(a) Water balance for all discharge taliks in the landscape



(b) Water balance for a discharge talik at the location of biosphere object 157_1

Figure 9. Water balance for taliks in the landscape (Figures A1-64 and A1-65 from Werner *et al.*, 2013).

Table 1. Net vertical groundwater fluxes (mm/y) for all groundwater-discharge taliks, biosphere object 157_1 and talik object 114. (From p140, Werner *et al.*, 2013).

Water-balance area	Object	Mire		Lake	
	Rock to Rego2	Rego2 to Rego1	Rego1 to surface	Rego2 to Rego1	Rego1 to surface
All discharge taliks	8	–	–	9	371
Biosphere object 157_1	31	–	–	31	375
Talik object 114	3	0	–3	4	7

Two talik areas are addressed in Werner *et al*. (2013). The particle tracking carried out in Bosson (2010) indicates that the 157_1 area would be a likely release area in the evolved landscape. As with the temperate cases there is detail for the entire landscape with resources then devoted to areas of less interest to the dose modelling (Object 114, for example, near the deep lakes to the northeast of the main release area at basin 157 is also discussed.) It is not clear if more detail could be added to the description of the talik-landscape around Object 157.

The dose assessment as described for example, on p35 of the biosphere synthesis report (SKB, 2014f) is based on a constant release rate, which is a basic limitation of the scenarios. Further, the MIKE-SHE modelling is basically quasi-steady-state even though the models are fed by time-series of precipitation and evapotranspiration reflecting seasonal variations. The relevance of that assumption depends on the aging of the talik (how rapidly it changes) and the duration of the scenario. According to SKB (2014c) taliks arise in a periglacial landscape (BCC2 scenario) at the end of a period starting from present climatic conditions until 17,500 CE, when the first 3,000-year period of cold climate arises. The change is done stepwise in the modelling. For a unit release, the assumption of quasi-steady state in the permafrost conditions might hold, but for a longer release as discussed on p130 of SKB (2014c) it may not.

The landscape development report R-13-27 contains nothing on permafrost development and taliks and very little on the effect of permafrost on sedimentation rates. What the report describes is the effect of land rise and sedimentation over millennia.

Overall then, it is clear that the overall talik description is at an earlier iterative stage that the temperate landscape. This was acknowledged by SKB (SSM, 2016b) and will be addressed in the next stage of assessment techniques.

3. Interpretation of FEPs in the landscape dose model

3.1. Overview

With each new dose assessment (SKB, 2008, SKB, 2011, SKB, 2014a) the process of iteration means that the models tend to accrete FEPs and that the FEPs become represented by different and usually improved mathematical descriptions as the database becomes ever more assessment specific.

The motivation for this review is to address how the new material has been identified and the representations justified. The scope of the SR-PSU dose assessment model is huge. The resources for the review preclude a detailed analysis of all of the facets of the dose assessment model. Fortunately the nature of the iterative process means that details in various parts of the SR-Site review material (Kłos *et al*., 2014; Kłos & Wörman, 2015) remain relevant. Where there are differences in SR-PSU – for example the increased vertical resolution in the regolith – these are well justified in the biosphere FEP analysis (SKB, 2013) and the mathematical description of the dose assessment model (Saetre *et al*., 2013a), notwithstanding the comments on the relation between the known stratigraphy and the translation of MIKE-SHE results of the dose model discussed in Section 2.2 of this report.

The full set of SR-PSU reports reviewed in this section comprises:

- Biosphere FEP analysis (SKB, 2013)
- Biosphere FEP handling (SKB, 2014b)
- Dose model description (Saetre et al. 2013a)
- Biosphere synthesis document (SKB, 2014c)
- Biosphere database (Tröjbom, et al., 2013; Grolander, 2013)
- Radionuclide transport and dose report (SKB, 2014d)

The scope of this part of the review has been to consider how the composite parts of the landscape dose modelling fit together, how they are identified and justified; how complete and informative is the documentation.

More focus is on the model for doses arising in the agricultural sub-models of the SR-PSU biosphere model. Invariably the agricultural doses are the highest for most radionuclides in the assessment. SR-PSU has modified the traditional concept of the "critical group" as members of subsistence communities to take into account historic lifestyles in the Swedish landscape (Saetre *et al*., 2013b). This is a significant improvement, in comparison to the approach used to define exposed groups in SR-Site (SKB, 2011), since it now relates lifestyles relevant to the possibilities of the landscape as expressed by the historical record. As noted in the previous section, there are some misgivings that the scope may not fully express the possibilities, however. There were no fishing lakes or dedicated fish farms historically. To fully explore the possibilities for exposure in the modelled landscape it might be considered prudent to extend such modern concepts to the description of potentially exposed groups. Alternate methods for defining exposure groups (Kłos & Albrecht, 2005) suggest that doses would unlikely to be as much as a factor of ten higher.

3.2. Documentation and traceability

There is a problem with the way material in the SR-PSU assessment it documented. Ideally there would be a clear path from FEP analysis to mathematical model derivation, description and illustration. Selection of the relevant data is included and there should be a clear indication of what the additional FEP brought into the assessment model at *this* iteration bring to the assessment. Results from the model as applied to the overall assessment are at the end of the process and the purpose of the documentation should be to provide traceability so that the quality of the approach can be verified.

In the SR-PU assessment all this material is available in the documentation. The problem is that the way it is documented is too fragmentary to be considered helpful. This is caused by the complete separation of the reports, as shown in the bullet points above. It is difficult to evaluate the modelling carried out when the mathematical expressions are in one place (Saetre *et al*., 2013a), the data in two reports (Tröjbom *et al*., 2013; Grolander, 2013), the evaluation of the results for limited deterministic cases and sensitivity studies are in in the synthesis (SKB, 2013), and the FEP handling report (SKB, 2014b) and the overall radionuclide transport and dose report (SKB, 2014d).

Where the documentation of the site descriptive material in SR-PSU is well structured, the same cannot be said of the documentation of the dose modelling.

The heart of the assessment is the numerical model – split into near- and far-field (nf/ff) modelling and biosphere modelling. The mathematical description of the landscape dose model and its implementation of FEPs (Saetre *et al*., 2013a) contains a lot of information. There is a reasonably clear correspondence between the FEP analysis for the biosphere (SKB, 2013) and the FEPs' mathematical description in Saetre *et al*., including an appendix giving an outline of the methods of compartmental modelling.

The compartment structures employed in the modelling are defensible and appropriate, although other interpretations are possible, as discussed in Section 2.2 above, in respect of the discretisation of the regolith. The complexity of the evolving landscape with changes to the geometry of the compartments is handled suitably. The results give a reasonable representation of *at least one* interpretation of the distribution of radionuclides in the regolith and water bodies of the *unperturbed* natural landscape.

It is reasonable to ask if alterative interpretations would lead to significantly different results but the relatively limited sensitivity studies reported in SR-PSU do not provide a comprehensive answer. There is scope for additional sensitivity analyses using both numerical techniques and alternate conceptual models.

The model's mathematical description uses a non-standard nomenclature throughout in both the documentation as well as the Ecolego models (made available as a result of the RFI). It is more usual for transfer processes in linear first order compartmental model representations to be written in the form of transfer rate coefficients, so that fractional transfer rate from the i^{th} compartment of the network to the j^{th} is described in terms of the fraction of the *inventory* of the radionuclide in the i^{th} compartment that is transferred in unit time: $\lambda_{ij} = \frac{1}{N_i}\frac{dN_{ij}}{dt}$ [year^{-1}].

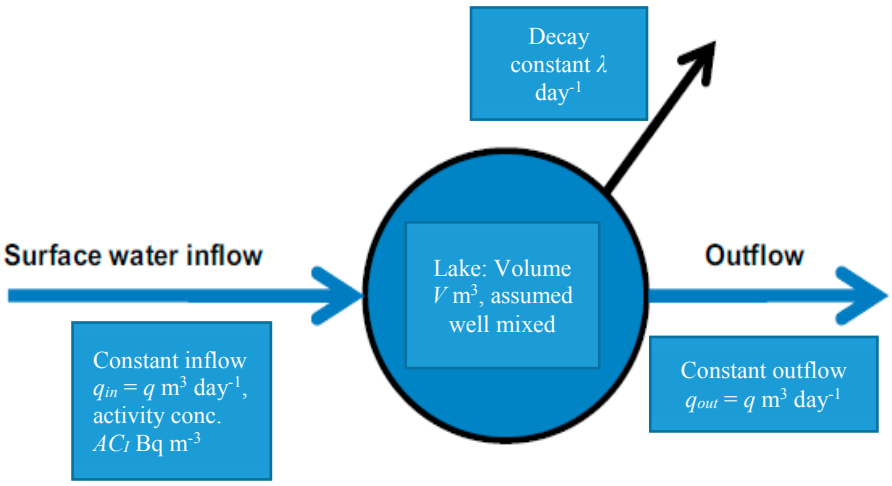


Figure 10. "Box and arrow representation of a hypothetical lake". Figure adapted from page 136 of Saetre *et al.* (2013).

Instead, the SR-PSU description uses the flux transferred, $\frac{dN_{ij}}{dt} = \lambda_{ij} N_i$ [Bq year^{-1}], ie, the "source term" from i^{th} to j^{th} compartment. This is not a major problem – the two representations are clearly isomorphic – except that it presents another obstacle in the path to true understanding, decreasing transparency. Appendix 1 of Saetre *et al*. provides an introduction to the "Principles of compartment modelling". It develops the ideas using the example of a simple 1-compartment model of a lake receiving activity from upstream (page 136, Figure A-1 reproduced here as **Figure 10**).

The rate of change of the activity concentration in the lake is given as

$$\frac{d}{dt}\left(V.AC_L\right) = q_{in}.AC_I - q_{out}.AC_L - \lambda\left(V.AC_L\right) \text{ Bq day}^{-1}.$$

The brackets correspond to the *inventory* in the lake water, $N = V.AC_L$ Bq, and it is a simple matter to rewrite the expression as,

$$\frac{dN}{dt} = S - \left(\frac{q}{V} + \lambda\right) N \text{ Bq day}^{-1}.$$

The quantity $\frac{q}{V} = \lambda_{outflow}$ day^{-1} is the transfer rate coefficient for outflow from the lake, expressed as standardised notation[3]. $S = q_{in}.AC_I$ is a *source term* for the lake.

The Appendix example is particularly trivial since so much is constant. This is presumably done to allow for a simple algebraic solution:

[3] Albeit with the rate expressed in units of day^{-1}, as with the decay constant in the example given.

$$\frac{N(t)}{V} = \frac{N_0}{V} e^{-\left(\frac{q}{V}+\lambda\right)t} + \left(1 - e^{-\left(\frac{q}{V}+\lambda\right)t}\right) \frac{q.AC_I}{q + V\lambda} \text{ Bq m}^{-3}.$$

Expressed as *concentrations* this is, as given by Saetre *et al*.

$$AC_L(t) = AC_L(0) e^{-\left(\frac{q}{V}+\lambda\right)t} + \left(1 - e^{-\left(\frac{q}{V}+\lambda\right)t}\right) \frac{q.AC_I}{q + V\lambda} \text{ Bq m}^{-3}.$$

There are therefore no real advantages to the change in formulation and it is not clear why the expressions have been written in this way. This convoluted approach to expressing the mathematical models is unnecessary and does nothing for clarity. The idea of setting out the basic principles is good but the result is not helpful in promoting understanding.

The example given is not at all representative of the generic set of FEPs in the landscape model. Working with concentrations as the means of expressing radionuclide transport lacks clarity when analysing with more complex systems. Using the inventory approach, the generic expression for the rate of change of the i^{th} compartment's inventory of radionuclide N (N_i Bq), taking into account the interactions with the j other compartments is

$$\frac{dN_i}{dt} = \left[S_i(t) + \lambda_N M_i + \sum_{j \neq i} \lambda_{ji}(t) N_j \right] - \left[\sum_{i \neq j} \lambda_{ij}(t) + \lambda_N \right] N_i \text{ Bq year}^{-1}.$$

The first term in first square brackets corresponds to external sources to the i^{th} compartment, the second is ingrowth from the parent radionuclide (M) in the i^{th} compartment and the summation term is the transfers into the compartment from the other compartments in the ensemble. The second square bracket represents the losses from compartment i due to radioactive decay and transport FEPs. This is significantly more detailed than the simple example in the Appendix of Saetre *et al*. The purpose is to *emphasise the detail*. First order linear dynamics are a powerful tool when applied correctly (there are restrictions imposed by the need to ensure homogeneity over spatial volumes for example), it is important to appreciate that though the mathematics is simple the systems can be large and complex – as in the case of the SR-PSU landscape dose model.

A simple expression of the model is

$$\dot{\mathbf{N}} = \mathbf{S} + \lambda_N \mathbf{M} + \mathbf{\Lambda N} \text{ Bq year}^{-1}.$$

This vector equation relates the changes in each of the compartments for the inventory of radionuclide N to each of the compartments in the system. Similarly the vectors **S** and **M** represent the external source term to each of the compartments and ingrowth. However, it is the transfer matrix, $\mathbf{\Lambda}$ year^{-1}, here that most succinctly expresses the dynamics of the landscape model. There are benefits to expressing the model in as few equations as possible.

Why does this matter? In a highly complex model such as the SR-PSU landscape model simplicity of documentation is important to transparency. Superfluous documentation hinders quality assurance. The system is complex – the example in Appendix 1 of Saetre *et al*. is trivial in comparison to the majesty of the entire model. If the landscape model could be expressed in such simple terms as that illustration the entire assessment would be much shorter.

The model is complex because the landscape is complex. The solutions to the equations of state are correspondingly not simple. There are irreducible complexities to the solutions that are not available from oversimplified systems. That is why the model is as it is. That is why tools such as Ecolego are used to obtain *numerical* solutions.

By doing so the assessment can focus on the impact of the FEPs, rather than concerning itself with *how to solve* the mathematics. Transparency would be aided by focusing on how to represent the FEPs in the simplest way possible, not on simplifying the mathematical representation of the FEPs to make the solution easy. This is discussed further in Section 3.3.2 on the modelling of cultivated soils.

3.3. Radionuclide transport modelling

3.3.1. Unperturbed landscape

From the site descriptive material discussed in Section 2 here, the landscape model is constructed to take into account water fluxes and landscape changes over the evolution of the site and out into the less dynamic landscape beyond around 10 kyear AP. The main focus of the landscape model is therefore to represent the evolution of the natural landscape and the fate of radionuclides released into it.

The landscape dose model is a natural progression from the SR-Site model of Avila *et al*. (2010) but with more detail and complexity, not least of which is the inclusion of ^{14}C as an important radionuclide in the source term for SFR.

The most significant developments in terms of the landscape evolution is that there are biosphere object-specific descriptions of the evolving hydrology to replace the region generic implementation in Avila *et al*. (2010). There are other important details – like the dynamics of peat growth that are added to the modelling. Another major difference is that in SR-PSU time dependent source terms are used in the evaluation of dose. Landscape Dose Factors (LDFs) are still employed in some parts of the model documentation and in some sensitivity analyses but the main SR-PSU assessment links biosphere to nf/ff models directly.

The most important feature of the landscape model as implemented is, of course, that it described an evolving landscape. Much of the detail in the model is therefore unavoidable since there is a need to express changes and conditions coded within the model that must be tested to determine which set of FEPs is active at the different times during the model run.

Many of these FEPs are updates of SR-Site and so represent a practical approach to the development of the landscape modelling methodology. However, the increased level of detail is potentially becoming something of a burden to the model. The fragmentary nature of the documentation and the multiple sensitivity analyses have not contributed to a demonstration that the landscape dose model is optimised for the purpose for which it is used. A well planned probabilistic sensitivity analysis would help rationalise the dose modelling, allowing simplification where possible and justifying the treatment of FEPs where necessary. Ideally this should be part of the overall documentation of the performance of the new, improved dose model. This issue should be addressed before the model becomes any more complex.

3.3.2. Doses from cultivated soils

In the main SR-PSU report the results show that the main ecosystem/lifestyle combinations for which the highest doses arise are associated with the drained-mire exposure group (Section 9.2, SKB, 2014a). This concentrates attention on how doses are calculated in this case.

Doses in the landscape dose modelling for natural – unperturbed – scenarios are calculated from the full expression of the regolith compartments (see Figure 6 for terrestrial compartments and their relation to the MIKE-SHE discretisation). Primary producers are included as dynamic compartments in the model. There are also additional processes include in the modelling of ^{14}C. The derivation of doses from the distribution in this landscape model is a reasonable and appropriate representation of the system.

As in SR-Site (Avila *et al*., 2010) doses from agricultural scenarios (*cultivated soils*) have a much simpler conceptualisation. The landscape dose model determines the radionuclide distribution in the unperturbed, natural, landscape. In the dose calculations from cultivation the radionuclide distribution from the landscape model is used to set the *initial conditions* for the cultivated soils. This corresponds to what has been identified as the accumulation-exposure scenarios for this type of landscape (Kłos, 2015a).

Cultivation of the natural soils in the Forsmark region requires emplaced drainage in the upper regolith (peat) with resulting compaction and, over a timescale of decades, oxidation of peat layers. These FEPs are better represented in the SR-PSU model that was the case in the Avila *et al*. model, a benefit of the iterative process.

In the Avila *et al*. model the agricultural soils were represented as a single compartment with an initial inventory. Activity in this compartment was then assumed to be leached as a results of net infiltration and this was criticised since it precluded the recycling of radionuclides from deeper regolith layers reaching the surface compartment as a results for the altered hydrology (Kłos *et al*., 2014). In SR-PSU the new model remains a single upper regolith compartment (with suitable properties) but with additional FEPs (see below for a detailed analysis). The cultivated soil model

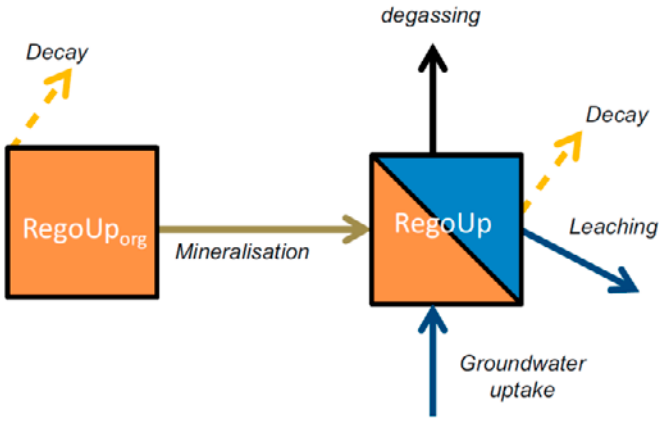


Figure 11. Agricultural soils in the Saetre *et al.* (2013a) model. Organic material from the mire (as peat) is converted to agricultural soil. Mineralisation implies conversion to "cultivated soil". The inventory in the soil undergoes losses by degassing (^{14}C) leaching and radioactive decay. There is a source term from the deeper regolith layers that serves to replenish the inventory. (Adapted from Figure 7-3 on page 77).

for the drained-mire exposure scenario is described in detail in Section 7.2.6 from page 82 of Saetre *et al*. (2013a).

Justification for single-compartment approximation used for cultivated soils (the *Inland-Outland* and *Garden-Plot* models are similar) would seem to be the assumption that cultivation over the same area of land, with such soil characteristics, is not likely to continue for an extend period. There is supporting evidence in Saetre *et al*. (2013b) for this. Over such a short period of time the transport processes would not be expected, especially for highly sorbing species, to redistribute activity to a high degree. The advantage of this simple interpretation is that, like the system described in Appendix 1 of Saetre *et al*. (2013a) a few more approximations mean that the system can be represented by a simple analytic solution which is then tacked onto the results for the landscape model to allow "agricultural" doses to evaluated at any time during the evolution of the unperturbed landscape model. The current Swedish regulatory guidance allows for the average dose over a 50 year period to be employed in determining dose. For comparison with the risk limit (SSMFS, 2008:21).

Figure 11 shows the conceptual model for the drained-mire system. The mire is organic material and this is drained for cultivation. There is progressive mineralisation that acts as a source term to the "soil" compartment (*RegoUp*) where it is leached and is subject to radioactive decay. The ^{14}C content of the soil can also degas to the atmosphere. From the deep regolith layers there is also an input.

In mathematical terms, the dynamic behaviour of the radionuclide inventory in agricultural soil after drainage can be described by the following system of ordinary differential equations given:

$$\begin{aligned}
\frac{d}{dt} regoUp_{org,DM} &= -\lambda.regoUp_{org,DM} - minRate.regoUp_{org,DM} \\
&= -\left(\lambda + minRate\right) regoUp_{org,DM} \\
\frac{d}{dt} regoUp^{RN}_{DM,i} &= GW^{RN}_{uptake,i} + minRate.regoUp_{org,DM} - \left(\lambda + k_{i,leach}\right) regoUp^{RN}_{DM,i} \\
\frac{d}{dt} regoUp^{^{14}C}_{DM,i} &= GW^{^{14}C}_{uptake,i} + minRate.regoUp_{org,DM} - \left(\lambda + k_{i,leach} + k^{^{14}C}_{degass}\right) regoUp^{^{14}C}_{DM,i}
\end{aligned}$$

In more conventional terms the relation the inventories in the organic compartment and the dry matter compartment are

$$\begin{aligned}
\frac{d}{dt} N_{regoUp,org,DM} &= -\left(\lambda_0 + \kappa_{regoUp,org,DM}\right) N_{regoUp,org,DM} \\
\frac{d}{dt} N^{rn}_{regoUp,DM,i} &= S^{rn}_{GW,i} + \kappa^{rn}_{regoUp} N_{regoUp,org,DM} - \left(\lambda_0 + k_{i,leach} + k^{rn}_{degass}\right) N^{rn}_{regoUp,DM,i}
\end{aligned}$$

This expression can be used for both the generic radionuclide and ^{14}C since for all radionuclides except ^{14}C, $k^{rn}_{degass} = 0$. The model expression simplifies from three equations to two.

λ_0	decay constant	year^{-1}	nuclide specific
$\kappa_{regoUp,org,DM}$	conversion rate of organic inventory to an inorganic inventory due to mineralisation	year^{-1}	nuclide specific

k^{rn}_{degass}	degassing rate	year^{-1}	nuclide specific (zero for all but ^{14}C)
S^{rn}_{GW}	"source term" from deeper soil	Bq year^{-1}	Assumed constant in the calculation of the 50 year average.

The leaching term is given as a standard transfer rate coefficient:

$$k_{i,leach} = \frac{(1-f_i) f^D_{regoUp,DM} \dot{I}_{agri}}{z_{drain,agri} s_{regoUP,DM} \varepsilon_{regoUp,DM}} \text{ year}^{-1}.$$

This expression can also be used for the ^{14}C model but for ^{14}C, $f_i = 0$. The parameters used in this expression are:

f_i	fraction of radionuclide inventory partitioned to the crop	Bq Bq^{-1}	nuclide and crop specific

$$f_i = \frac{K_i B_{DM,i}}{K_i B_{DM,i} + z_{drain,agri} \rho_{b,regoUp,DM}}.$$

The use of the soil-plant CR for the i^{th} crop type relates the inventories in the soil and crop (with double counting of the fraction in the crop),

K_i	CR for crop *i*	Bq Bq^{-1}	Nuclide and crop specific
$B_{DM,i}$	Biomass of crop *i*	kgC m^{-2}	Crop specific
$z_{drain,agri}$	Depth of top soil	m	Ecosystem specific
$\rho_{b,regoUp,DM}$	Bulk density of top soil	kg m^{-3}	Ecosystem specific.

There is also an expression for the "fraction of the radionuclide in solute phase":

$$f^D_{regoUp,DM} = \frac{1}{1+\frac{K_{d,regoUp,DM}\rho_{b,regoUp,DM}}{s_{regoUP,DM}\varepsilon_{regoUp,DM}}} = \frac{s_{regoUP,DM}\varepsilon_{regoUp,DM}}{s_{regoUP,DM}\varepsilon_{regoUp,DM} + K_{d,regoUp,DM}\rho_{b,regoUp,DM}}$$
$$\equiv \frac{\theta_{regoUp,DM}}{\theta_{regoUp,DM} + (1-\varepsilon_{regoUp,DM})\rho_{regoUp,DM} K_{d,regoUp,DM}},$$

a quantity better known as the "retardation factor" – see Appendix A of Kłos *et al*. (1996).

There is a form of time-dependent "source term" from the deeper soil of the drained mire. In the 50-year average calculation it is apparently constant (page 82) but on page 80 the general expression is discussed:

$$GW^{rn}_{uptake} \equiv S^{rn}_{GW,i} \equiv \dot{I}_{sat\rightarrow unsat,agri} f_{area,i} A_{DM} N_{group,DM} C^{D,rn}_{soil,Sat}.$$

The parameterisation is

$\dot{I}_{sat\rightarrow unsat,agri}$	Flux from saturated to unsaturated	m^3 m^{-2} year^{-1}	*Where does this numerical value originate? Is it in Grolander?*

A_{DM}	Area of "drained mire"	m^2	
$f_{area,i}$	Fraction of total object area used for crop *i* production. For ^{14}C this is set to unity.	unitless	This distinguishes the standard model from the ^{14}C model.
$N_{group,DM}$	Number of individuals in the exposed group	persons	Object specific.
$C^{D,rn}_{soil,Sat}$	Concentration in the deeper layer	Bq m^{-3}	Variable depending on the scenario considered. Really rather complex.

For this case the initial conditions in the soil layers are defined on page 78 in terms of the inventories at the specific time for which doses from the agricultural model are to be calculated.

In general terms the two equations to be solved are (dispensing with the DM label)

$$\frac{dN_{org}}{dt} = -\left(\lambda_0 + \kappa_{org}\right) N_{org}$$
$$\frac{dN_i}{dt} = S_i + \kappa_{org} N_{org} - \left(\lambda_0 + k_{i,leach} + k^{rn}_{degass}\right) N_i .$$

The drained-mire (DM) case starts with an inventory in the organic compartment. This mineralises over time so that

$$N_{org}\left(t\right) = N_{org}\left(0\right) e^{-\left(\lambda_0 + \kappa_{org}\right)t} .$$

In turn, then

$$\frac{dN_i}{dt} = S_i\left(t\right) + \kappa_{org} N_{org}\left(0\right) e^{-\left(\lambda_0 + \kappa_{org}\right)t} - \left(\lambda_0 + k_{i,leach} + k^{rn}_{degass}\right) N_i$$
$$\frac{dN_i}{dt} \equiv S_i\left(t\right) + \kappa_o N_o e^{-\left(\lambda_0 + \kappa_o\right)t} - \left(\lambda_0 + \kappa_i\right) N_i$$

provides the simplification of notation. The integral is then

$$\int_{N_i(0)}^{N_i(t)} \frac{dN_i}{S_i\left(t\right) + \kappa_o N_o e^{-\left(\lambda_0 + \kappa_o\right)t} - \left(\lambda_0 + \kappa_i\right) N_i} = \int_0^t dt = t .$$

There is no *exact* analytical solution for this – as there was for the even simple single compartment agricultural soil model in the SR-Site calculations (which neglected recycling from the deep soil). The solution quoted on page 83 of Saetre *et al*. corresponds to

$$N_i\left(t\right) = N_i\left(0\right) e^{-\left(\lambda_0 + \kappa_{degass} + k_{i,leach}\right)t} + \left\langle S \right\rangle \frac{\left(1 - e^{-\lambda_0 + \kappa_{degass} + k_{i,leach} t}\right)}{\lambda_0 + \kappa_{degass} + k_{i,leach}}$$
$$+ \kappa_{org} N_{org}\left(0\right) \frac{e^{-\left(\lambda_0 + \kappa_{org}\right)t}}{\lambda_0 + \kappa_{degass} + k_{i,leach}} \left(1 - e^{-\left(\lambda_0 + \kappa_{degass} + k_{i,leach}\right)t}\right) .$$

where the time varying source term, $S_i(t)$, is replaced by a constant value, $\langle S \rangle$, averaged in some unspecified way.

As discussed previously, it would make as much sense to have a numerically integrated expression as a side calculation to the main landscape model. In discussion with SKB (SSM, 2016b) it seems that such an option for future iterations us being considered.

4. Probabilistic modelling in SR-PSU

4.1. Implications of chemical evolution of soils

The chemical properties of the soils at Forsmark are strongly influenced by the high $CaCO_3$ content (page 40, SKB, 2014c). The soils are relatively immature and the carbonate content is expected to decline over time,

> *Most of the easily weathered calcite in the upper regolith of the Forsmark area will be dissolved and ultimately washed out over time. This means that the influence of the calcium-rich deposits on freshwater and the terrestrial ecosystems will be reduced. Thus, the future chemical environment in the area is expected to approach the low-calcite conditions more common in Sweden, implying a pH drop between one and 1.5 units in freshwater and wetlands/agricultural soils when data from Forsmark are compared to areas low in calcite.*

(page 218, SKB, 2014c). Rather than modelling the evolution of carbonate content directly SKB (2014c) explains that the uncertainty introduced to the modelling as a results of the leaching was handled in the models *by allowing the probability density functions of pH sensitive parameters to span the expected response to a decrease in pH*.

The question is, does it make a difference to the results that the distribution is used as a surrogate for the evolution of the soil chemistry. A short modelling exercise has been carried out to address this issue.

We have no specific model for the SR-PSU objects so a simple interpretation using GEMA-Site, SSM's SR-Site model (Kłos, 2015a) has been adopted as a generic Forsmark basin.. The effect on the concentration in unperturbed (ie, remaining in the natural undrained state) wetland soils at the end of a 10 kyear simulation is evaluated using a k_d for the soil upper regolith compartment that changes linearly with time. The result is compared to the mean concentration obtained with a constant soil k_d sampled using the SR-PSU pdf in a probabilistic calculation.

The intention is not to redo any of the SR-PSU calculations, rather the aim is to investigate the suitability of SKB's chosen method for addressing the issue. To this end the GEMA-Site model for the SR-Site independent calculation adopted with only changes to the top soil k_d modified. The radionuclides selected for the study are ^{129}I (relatively mobile) and ^{94}Nb (relatively immobile). The relevant SR-PSU k_d is K_d_regoUp_ter for the *compartment represents the upper oxic layer of terrestrial*

Table 2. Solid-liquid distribution coefficient used to evaluate the impact of time-dependent k_d modelling on the concentration of radionuclides in upper regolith soils. The values for Kd_regoUp_ter are given on page 84 of Tröjbom *et al*. (2013) as translated into the model "LandscapeMainChain_CC1.eas" provided by SKB following the RFI.

Radionuclide	^{129}I	^{94}Nb
K_d	K_d_regoUp_ter m^3 kg^{-1} dw	
Pdf	truncated lognormal	
BE	0.20374336	7.277983643
GM	0.20374336	7.277983643
GSD	3	3
lower truncation	0.033436	1.1943912
upper truncation	1.24150346	44.3481532

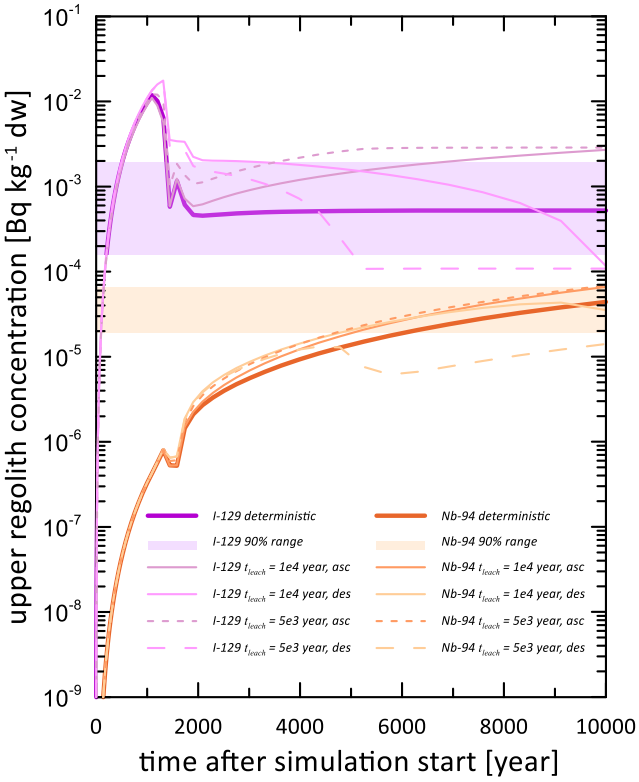


Figure 12. Simulating the effect of time varying soil k_ds by sampling from a defined range. The range of probabilistic results for the concentration at 10 kyear of ^{129}I (purple) and ^{94}Nb (orange) are compared with results from a deterministic case (constant k_d) and cases with time-varying ()both *inc*reasing and *dec*reasing k_ds with different $CaCO_3$ leaching times.

regolith (peat). This uppermost layer is biologically active, with relatively high rates of decomposition and root activity. The depth of the layer is fairly constant (c.10 cm) and limited by the diffusion of oxygen (Saetre *et al*. 2013a).

Table 2 shows the numerical data used. For this evaluation we assume that the truncation values represent the full range expressed as a consequence of the leaching of $CaCO_3$ and it is consistent with SKB's use of parameter distributions to simulate the effect of sorption.

Depending on the k_d value that corresponds to high or low $CaCO_3$ content, the time varying k_d is given by increasing k_d with time

$$k_d(t) = \begin{cases} k_{max} & t > t_{leach} \\ k_{min} + \dfrac{k_{max} - k_{min}}{t_{leach}} t & t \le t_{leach} \end{cases}$$

or

$$k_d(t) = \begin{cases} k_{min} & t > t_{leach} \\ k_{\max} - \dfrac{k_{max} - k_{min}}{t_{leach}} t & t \le t_{leach} \end{cases},$$

when the k_d decreases over time.

The other variable here is the leaching time, the time taken for the effective removal of $CaCO_3$. The simulation runs for 10 kyear and results for leaching times of 5 and 10 kyear are evaluated.

The model used is that reported in Kłos (2015a) for a small basin with geometry such that the areas of the outer, inner and central parts of the basin are in the ratio $10^5 : 10^4 : 10^4$ m^2 (see Kłos 2015b). A modified model for this purpose has been created. Starting from the shallow sea situation of the present day (depth assumed to be around 10 m at the centre of the basin, the transition to bay status is assumed when the sea level is reduced to 2 m. A unit release of each radionuclide is considered.

The results in Figure 12 show that the ranges from the probabilistic simulation (shaded areas) correspond reasonably well to the results when the k_d of the upper regolith is varied. This result supports SKB's interpretation in SR-PSU that the time variation of soil chemistry can be reasonably well approximated by the simple expedient of employing a range of k_d values. However, it should be noted that there are many other parameters in the Saetre (2013a) models relating to carbonate content and that the radionuclides considered here have not included ^{14}C.

4.2. Probabilistic Sensitivity Analysis in SR-PSU

4.2.1. Combination of Sample sets in the SR-PSU sensitivity analysis

One of the RFIs concerned the number of distinct sample sets for the biosphere calculations compared to the combined calculations for the near-field/far-field (nf/ff) models. The discussion at the April 2016 meeting at SSM between SKB SSM and reviewers clarified the approach.

Because of high run times for the combined near-field/far-field models 100 sample sets were generated for these and the results used as input to the biosphere model. The biosphere sample set comprised 1000 datasets. The 100 nf/ff sets were therefore each reused 10 times to match the overall biosphere sample sets to give statistics based on 1000 sample sets.

However, the formulation of the total system sensitivity study reported in Appendix F of SKB (2014d) is difficult to ascertain; for the biosphere parameters sampled there is a reference back to the discussions in Grolander (2013) for the biosphere parameters and to the data report (SKB, 2014e) so that the fragmentation of the documentation again causes problems for traceability. The sensitivity analysis dose calculations involved "several hundred parameters have been varied according to prespecified probability density functions". SKB (2014d) states (on page61) that

> *Monte Carlo simulations with Latin-hypercube sampling … were performed using 100 iterations for the near-field and far-field. The data set from these*

Table 3. Statistics for calculated (retardation coefficient, R) and input (soil K_d)for LHS 1000 and 100 sample sets and the combined case where the 100 LHS samples were recombined with the full 1000 samples for the porosity and density in the evaluation of R.

	Retardation coefficient			Deep soil K_d		
	LHS 1000	LHS 100	combined	LHS 1000	LHS 100	combined
mean	6.4E+03	5.2E+03	6.6E+03	1.8E+01	1.9E+01	1.9E+01
GM	2.5E+03	2.5E+03	2.5E+03	1.3E+01	1.3E+01	1.3E+01
GSD	4.2	3.1	4.2	2.4	2.6	2.4
5th%	2.5E+02	2.2E+02	2.2E+02	3.1E+00	3.1E+00	3.1E+00
95%	2.6E+04	2.2E+04	2.6E+04	5.4E+01	5.3E+01	5.3E+01

calculations was used as input to Monte Carlo simulation of the biosphere and dose calculations, using 1,000 iterations.

It is important the LHS sampling was used for the nf/ff combination since the purpose of Latin-Hypercube sampling (LHS) is to ensure an adequate coverage of parameter space for the individual model components in a way that simple Monte Carlo (MC) sampling cannot for small sample sizes (see Campolongo *et al*. 2000). LHS is a form of MC sampling but it is important to make the distinction. MC would probably not provide adequate coverage of the sample space for the near- and far-field model.

What remains in question of the adequacy of using 100 nf/ff sample sets repeated 10 times each with the 1000 sample sets of the biosphere model. To address this issue a greatly simplified "model" is employed. Consider the retardation coefficient for the deep soil compartment, in the form

$$R = \varepsilon + (1-\varepsilon)\rho k_d \ ,$$

where the medium is saturated and the retardation depends on the porosity (ε , unitless), grain density (ρ kg m^{-3}) and the solid distribution coefficient (k_d m^3 kg^{-1}). Using this as an analogue for the combination, where porosity and density are sampled 1000 and 100 times (pdfs for porosity and density are taken from the Grolander (2013) database and Tröjbom *et al*., (2014) for the k_d of ^{94}Nb.

Table 3 shows the statistics for the retardation coefficient calculated for each of the 1000 and 100 LHS cases, the combined dataset, where the 100 samples for K_d in the 100 LHS dataset are repeated ten times.

While not a conclusive result, since the modelled system is rather simple here, this finding lends support to the approach taken by SKB. A more complete demonstration from SKB would be welcome.

4.2.2. Output quantity

In SKB (2014d) the quantity carried forward to the risk evaluation is defined on page 61:

> *Exposure to these representative individuals is considered in several potentially contaminated biosphere objects. The maximum dose across all land-use variants and biosphere objects at each point of time is the most important presented time-dependent performance indicator for a calculation case.* ***The maximum over time of this maximum dose defines peak dose, which is the quantity carried on to the risk assessment***,

emphasis added.

Chapter 5 of SKB (2014d) goes on to discuss the results in terms of several time series for radiotoxicity and dose. Both quantities are presented as arithmetic mean values. The plots suggest that the quantity used to determine dose is the time series of average combined dose over all realisation, $\langle D_{tot}(t) \rangle$ Sv year^{-1} and the quantity compared to the risk criterion derived dose is then $\max \langle D_{tot}(t) \rangle$.

This quantity may not fully represent the dose. Averaging over a number of simulations for which the time of the peak dose might vary would imply that $\max \langle D_{tot}(t) \rangle$ might be lower than a similar quantity, $\langle \max D_{tot}(t) \rangle$ Sv year^{-1}. This is the mean of the peak dose in each of the simulations, irrespective of the time of occurrence.

However, it is likely the difference between the two quantities is small in this case. As SKB (2014d) notes: *the dynamics of the maximum annual dose curve … mainly reflects the dynamics of radionuclide releases from the repository*. The biosphere perturbs the release dynamic only slightly but the variation in the release curves in the 100 nf/ff sample sets could have an effect that this not investigated in SR-PSU. Nevertheless the preferred usage of averaging should be clarified.

5. Discussion

The BIOMASS methodology (IAEA, 2003) set out seven steps in the process of developing biosphere models for dose assessment *for each iteration*. Only the assessment context is unlikely to change between iterations. As seen in the documentation of SR-PSU there has been considerable development since the last assessment of SFR as well as significant re-interpretation of material from the SR-Site assessment. At each iteration step in the sequence, the place where the new material needs to be integrated depends on the nature of the material.

In SR-PSU the increased timescale of the assessment compared to previous two dose assessment model iterations means that some review of the biosphere system identification and justification was required, for example with the introduction of periglacial systems into the landscape dose modelling for the first time. The biosphere system description now includes a development of hydrological modelling for specific objects and there has been a review of the representation of potentially exposed groups to take into account a more detailed description of historically-based lifestyles in Sweden. Consequences for the conceptual and mathematical models arise from the new material. In particular for ^{14}C there has been a complete revision of how the radionuclide transport accumulation and dose is modelled since the previous SFR assessment. The ^{14}C model is now integrated with the other radionuclides in the dose assessment models.

A key feature of the BIOMASS methodology is identification and justification. Though expressly stated prior to the definition of the *biosphere system description* in the methodology it can – and should – equally apply to the model development. There is a need to identify the required FEPs for the model (adequately addressed in

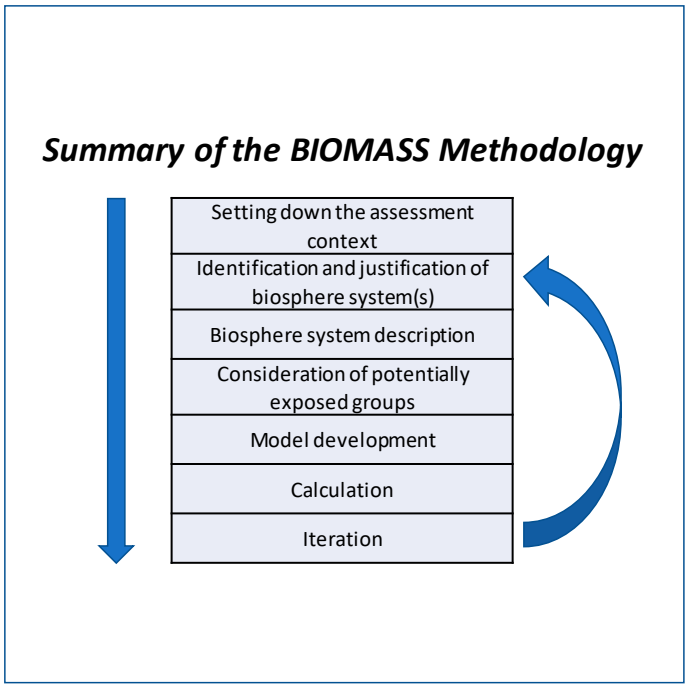


Figure 13.Summary of the BIOMASS methodology for developing assessment-level biosphere dose model (modified from IAEA, 2003).

the SR-PSU documentation) and the justification of the way in which they are implemented. In the SR-PSU documentation this is not adequately done. It requires that the behaviour and characteristics of the new iteration's model be demonstrated and that the benefits of the revised approach to the assessment be clearly demonstrated.. This is not done in the SR-PSU documentation. As discussed above, the piecemeal approach to documentation means that a comprehensive understanding of the performance of the resulting landscape dose model is difficult to achieve. The missing ingredient is the documentation of model performance, specifically of the landscape dose model.

It could be argued that the landscape dose model in SR-PSU is a straightforward upgrade of the model used in the SR-Site dose assessment and as such does not require a thorough illustration of its capabilities. This does not take into account the significant differences in the way in which ^{14}C is modelled in SR-PSU compared to the corresponding assessment for the SFR repository in SAR-08 (SKB, 2008).

There are also interactions between the hydrological description and other parts of the model to consider. The representation of hydrologically distinct mire/wetland on the one hand and lake systems on the other. Transfer only in the upper regolith (see Figure 6), is a modelling choice where the implications need further investigation. Similarly, that the upper regolith of the 157_2 mire area only transfers activity to the upper regolith of the 157_1 mire area also presents some scope for alternative interpretation. The revision of the SR-Site hydrological modelling (using a generic representation of the hydrologically distinct basins) to a more object specific approach is a clear improvement but it is the set of modelling assumptions in the dose assessment model itself that is of concern here.

For radionuclides other than ^{14}C the assumption is reasonably cautious since the assumption retains activity in the 157_2 object. The dynamics of ^{14}C are rather different in the new model. In particular the role of the *piston velocity,* that acts to degas the ^{14}C content of the upper regolith, is clearly important in reducing the inventory of ^{14}C in the 157_1 lake.

Degassing from the top regolith layer is given by (page 65, Saetre, *et al*., 2013a)

$$\frac{dN^{D14C}_{\mathrm{Re}goUp,ter}}{dt} = f_{H_2CO_3,ter} v_{pist,ter} A_{ter} C^{D14C}_{\mathrm{Re}goUp,ter} \text{ Bq year}^{-1},$$

where

$C^{D14C}_{\mathrm{Re}goUp,ter}$ Bq m^{-3} activity concentration of ^{14}C in dissolved porewater,

$$C^{D14C}_{RegoUp,ter} = \frac{N^{D14C}_{RegoUp,ter}}{\theta_{RegoUp,ter} l_{RegoUp,ter} A_{ter}} \text{ Bq m}^{-3},$$

so that

$$\lambda_{degas} = \frac{1}{N^{D14C}_{RegoUp,ter}} \frac{dN^{D14C}_{RegoUp,ter}}{dt} = \frac{f_{H_2CO_3,ter} v_{pist,ter}}{\theta_{RegoUp,ter} l_{RegoUp,ter}} \text{ year}^{-1}.$$

The parameters are

$f_{H_2CO_3,ter}$	Bq Bq^{-1}	is the fraction of dissolved inorganic carbon that is in the form of CO_2 / H_2CO_3 in pore water of surface peat - uniform (0.46, 0.03, 0.96) (page 95, Grolander, 2013)
$v_{pist,ter}$	m year^{-1}	is the gas exchange coefficient for peat in contact with the atmosphere (i.e. the height of the upper peat layer that is equilibrated with the atmosphere per unit time) – uniform (50, 45, 55)
$\theta_{RegoUp,ter}$	-	is the volumetric moisture content of the soil layer (assumed saturated and equal to porosity, $\varepsilon_{RegoUp,ter}$, of the wetland area). Grolander (2013) page 46 – uniform (0.9, 0.88, 0.94)
$l_{RegoUp,ter}$	m	thickness of the upper regolith layer.

Downstream loss via surface drainage

$$\lambda_{drainage} = \frac{F_{drainage} + k_{RegoUp,ter} M_{drainage}}{\theta_{RegoUp,ter} l_{RegoUp,ter} R_{RegoUp,ter}} \text{ year}^{-1}$$

Is in the standard form for liquid and solid transfers (for which we assume here $M_{drainage}$ = 0) so the ratio of degassing losses to drainage losses is

$$\frac{\lambda_{degas}}{\lambda_{drainage}} = R_{RegoUp,ter} \frac{f_{H_2CO_3,ter} v_{pist,ter}}{F_{drainage}}.$$

Obviously, for those radionuclides that don't degas, this is zero. For ^{14}C, however, the ratio depends on the retardation coefficient

$$\frac{\lambda_{degas}}{\lambda_{drainage}} = \left(1 + \frac{\rho_{bulk,RegoUp,ter}}{\varepsilon_{RegoUp,ter}} k_{RegoUp,ter}\right) \frac{f_{H_2CO_3,ter} v_{pist,ter}}{F_{drainage}}$$

$\rho_{bulk,RegoUp,ter}$	kg m^{-3}	bulk density of wetland soil, p. 46, Grolander (2013) – uniform (100, 65,136).

For ^{14}C there is no retardation (k_d = 0) so we have $\frac{\lambda_{degas}}{\lambda_{drainage}} = \frac{0.46 \times 50}{F_{drainage}} = \frac{23}{F_{drainage}}$.
Even taking the whole net precipitation ($P - E$) as the water flux from the upper layer, the piston velocity trumps everything.

However, page 97 of Grolander expresses some of the difficulties with the model, noting that the piston velocity derived from experiments might be an overestimation so that the value actually used is reduced by a factor of three because *compared with empirical estimates, suggested that the degassing of CO_2 was too effective in the model (SKB 2014a, Chapter 9)*.

Therefore, the role of the piston velocity is crucial in removing activity from the upper regolith of 157_2 – the only compartment that interacts downslope with 157_1 – so that there is very little ^{14}C in the upper regolith to be transferred downslope to the 157_1 lake.

What if the subsurface flows in Figure 6 were to be included in the transfer processes between the 157_2 and 157_1 mire and lake objects? Would the contribution to dose from ^{14}C be higher?

From the regulatory guidance document (SSMFS, 2008:37),

> *Reporting should be based on a quantitative risk analysis in accordance with the advice on Sections 5 to 7. Supplementary indicators of the repository's protective capability, such as barrier functions, radionuclide fluxes and concentrations in the environment, should be used to strengthen the confidence in the calculated risks.*

In this case, particularly when a new model is introduced, it is necessary to explore and support the assumptions with *supplementary* analysis. This has not been carried out sufficiently in SR-PSU. In terms of the BIOMASS methodology there has been a great deal of identification and justification of the system description. The site descriptive modelling and understanding is becoming mature as a discipline at SKB, but further development of the landscape modelling techniques is required.

As far as can be determined by this review of the SR-PSU documentation and supplementary material from the RFI response there are no obvious omissions from the SR-PSU assessment. The doses calculated are credible and the methodology is broadly appropriate. The only misgivings come from the decreasing completeness of the documentation as the reports move from the well documented site descriptive material to the details of the dose assessment modelling and how this is integrated into the overall assessment. There are a number of instances where supplementary analyses should have been carried out to support the main findings. Alternative conceptual models and implementation would help build confidence in the SR-PSU results. Some of these issues have been recognised by SKB and are expected to be addressed in the next iteration of SKB's assessment modelling for both the low and intermediate level repository and the planned spent fuel repository at Forsmark.

6. Conclusions

Overall impression – landscape modelling in the SR-PSU assessment
There is nothing in the main phase review of landscape modelling for the SR-PSU dose assessment that would suggest that the results are inappropriate. There are, however, a number of reservations relating to both the breadth of the biosphere dose assessment and the overall documentation of SR-PSU, with particular respect to dose assessment modelling.

SKB have acknowledged some of the issues raised during the review as subjects for further development in future modelling and assessment iterations of both the SFR3 for radioactive decommissioning waste and of the deeper repository for spent fuel, both at Forsmark. Suggestions for outstanding issues are set out below.

Scope of the main phase review
The initial review phase (SSM, 2016) focused on the higher level reports, main SR-PSU report (SKB, 2014a) and the biosphere synthesis report (SKB, 2014c). In this main phase of the review the lower level reports (hydrology, landscape development, model, nuclide specific and other data: respectively Werner *et al*., 2014; Brydsten & Strömgren, 2013; Tröjbom *et al*., 2013 and Grolander, 2014) have been covered in greater detail together with other material, specifically the information provided by SKB in response to the Requests for Further Information (RFIs) that were communicated to SKB at the end of the initial phase.

Suitability of the reported biosphere modelling
The overall conclusion is that results from the landscape modelling are credible and appropriate but the sensitivity analyses carried out do not give a sufficiently broad expression of the possibilities for exposure in the future landscape. There needed to have been follow up calculations to support the main model results and conclusions. This would have added weight and enhanced confidence in the overall assessment results.

The dose assessment model is overly complex and an optimisation strategy should be implemented. The landscape dose model should remain the main dose assessment modelling tool but not the only one. Simpler models should be used to illustrate points of significance. This is similar to the approach taken in the current assessment, where the models for doses arising from agricultural soils (the ecosystem dominating the peak dose results) are much simpler than those in the main landscape model but rely on the landscape modelling to set initial conditions. A case could be made for the main landscape model to be used as the radionuclide transport and accumulation model for the unperturbed, natural system (lakes, seas, bays, forest, wetland) with doses calculated as required for specific potentially exposed groups. For exposure groups associated with changes to the natural system (specifically agriculture and cultivation) additional models, or exposure scenarios might be considered so as to build confidence. Currently the perturbed models are integrated with the main unperturbed model with a subsequent lack of clarity. The above approach would allow for more scoping studies to be addressed. An example is the potential for a small fishing pond within the boundaries of Object 157_2. There may well be good reasons to rule out such a feature of the future landscape but the issue needs to be clearly addressed.

The biosphere safety analysis identified potential issues but did not take them any further, for example, the interpretation of the landscape at 157_2 and the potential for the transport of ^{14}C from the mire to the lake before degassing could significantly deplete the inventory of the upper regolith. A more comprehensive review of the be-

haviour of radionuclides in the whole of basin 157 should be carried out with particular reference to the evolution of the objects around the time of transition from bay to terrestrial ecosystems. This would help confirm the findings of the SR-PSU assessment. Essentially this suggestion corresponds to a refocussing from the whole landscape of the site descriptive modelling to the key areas in the dose assessment modelling.

In the SR-PSU biosphere dose modelling the comprehensive detail of the site descriptive material exerts a strong influence on the format and function of the dose modelling. This leads to a somewhat prescriptive expression of the future evolution: there is one regolith-lake development model. There is one set of release locations used to define the morphology of the dose model objects and hence their hydrology. The various sensitivity studies (a mixture of deterministic and probabilistic) are discussed over several documents which means that the integration of relevant discussions is weak. In this respect the biosphere synthesis document and the radionuclide transport report (respectively SKB, 2014c and SKB, 2014d) give slightly conflicting results.

This overly prescriptive view of the future of the landscape arises from the detailed site descriptive modelling being used to determine what the dose assessment model can consider rather than the dose assessment model informing the site descriptive modelling what needs to be better understood. The balance between these two requirements has improved since SR-Site (with the review of the definition of the potentially exposed groups) but more is required in the future iterations of dose assessment modelling for both spent fuel as well as for SFR, beyond SR-PSU.

Documentation and iteration
A major difficulty in carrying out the review has been the disjoint nature of the documentation. Individually the reports are of good quality. The synthesis is less persuasive. Not all of the relevant material in the lower level reports (R-reports) has been carried forward to the synthesis. Because the different reports have different roles, the review is made more complex. For example when reading the description of the dose assessment model (Saetre *et al*., 2013a) it is difficult for the reader to integrate the model description into the overall assessment because data are reported in one place with results in an entirely different document. The role of the synthesis document should have been to bring this material all together. Because the different parts were separate this was not successfully achieved. Perhaps because of the late appearance of the biosphere FEP report (SKB, 2014b) some of the potentially important information in the sensitivity analysis was not followed up in the DEM sensitivity studies, for example the potential role of the vertical discretisation of regolith in the MIKE-SHE calculations.

There is a perceptible gradient of detail and quality from the SDM to the dose assessment model. Much of the SDM is material that was under development at the time of SR-Site and has reached a level of maturity at this assessment. The assessment process is one of continuous iteration. There is always new material to be added to the understanding of the site and its evolution. This must be embedded in the dose assessment modelling. The first approximation to describing evolving basin-hydrology in the SR-Site dose assessment model has been replaced by a more detailed and basin specific interpretation.

The longer assessment timescale for which detailed models of the system evolution means that state changes between temperate and periglacial climate conditions are now explicitly included in the assessment model sequence. Treatment of periglacial conditions as part of the overall evolutionary sequence is now that part of the modelling which is less well defined. This is acknowledged as such by SKB (in comments reported by SSM, 2016b) and is expected to be further developed. Those parts of the

documentation that have featured in earlier assessments are therefore well documented. Where the quality of the documentation begins to falter is in the translation and interpretation of the extensive site descriptive modelling to the performance assessment model.

Where there is a detailed description of surface systems with many possible interpretations, only a single interpretation of the regolith-lake development model (Brydsten & Strömgren, 2013) is carried forward to the site description on which the dose assessment model is based. As noted by SKB (in SSM, 2016b) the overall perturbation to the new DEM derived for SR-PSU (Strömgren & Brydsten, 2013) are small when comparing the bathymetry around the key release areas in the DEM and the expected *topography* at future times. It can therefore be argued that some scope for alternative interpretations of landscape and human interaction are appropriate at this iteration. The single interpretation in SR-PSU is too restrictive.

The fragmentary structure of the documentation does not help in this respect. While the individual reports are self-contained and, seemingly, complete, a wider perspective with the aim of integrating all the documents suggests that the quality gradient from SDM to assessment model means that confidence in the assessment results is not as high as it could be. The means to address these issues are discussed in the recommendations below.

In respect of the biosphere dose modelling, the biosphere synthesis document (SKB, 2014c) can be seen to be ineffective. In part this is because of the discretisation of the documentation. The R-level reports

- Model description (Saetre *et al*., 2013a)
- Data interpretation (Grolander, 2013)
- Nuclide specific data (Tröjbom *et al*., 2013)

each discuss distinct aspects of the assessment modelling. These are substantial reports and it is difficult to integrate their contents individually. There needs to be a context. This might be the biosphere FEP report (SKB, 2014b) which discusses the *handling of biosphere FEPs and recommendations for model development in SR-PSU*. The late appearance of this particular publication meant that an important subset of information needed for the initial review phase was absent. Moreover, potentially important interpretations of the hydrology of basins were not available since they were not carried forward to the biosphere synthesis document.

Recommendations
Moving forward from SR-PSU there are two areas that need to be better expressed in SKB's future dose assessment models. These are outlined below.

Simplified dose modelling

- A central role for landscape model is confirmed treating it as the reference implementation for radionuclide transport and accumulation in the unperturbed system and linked directly to the site descriptive material. The detailed evolving radionuclide transport model could therefore be interpreted as an intermediate step in the estimation of doses. A decoupling of the transport modelling from the dose calculations might be considered.
- Treating the doses calculations independently from the transport modelling would promote a review of potential submodels for exposure (agriculture, cultivation/kitchen garden, fish farm, etc.) should be considered. A FEP re-

view focussing on *potential exposure scenarios* is needed to enable the assessment team to think beyond the constraints of the locus of the site descriptive modelling.
- A rationalisation of the landscape and dose models is required. A large number of FEPs have been added to the SR-PSU dose assessment models. The results of the SR-PSU sensitivity studies do not show them as important to dose. The aim should be to avoid the baroque monarchy approach and to adopt a Spartan meritocracy (see SSM, 2016a, after Haldane, 2003).
- A detailed look at transients in the key release area of 157 as the shoreline retreats and in the approach to steady-state flow conditions.
- Detailed review of alternative hydrology that could lead to transport of ^{14}C in wetland soils in 157_2 to the lake in 157_1 before depletion by degassing.

Better documentation
A better integrated set of documents is needed. It is acknowledged that this is difficult for such a large project. However it is essential that model descriptions include some indication of how the model performs (requiring illustrative examples and practical sensitivity studies). Documentation of the effects of newly introduced FEPs is important. Comparison with model results at the earlier iteration is therefore required.

A better way of illustrating the link between model results and the datasets used for a particular run is needed. In the SR-PSU documentation the traceability of results and datasets was very difficult. This hindered transparency and made independent reproduction of results difficult.

Two matters already identified in the initial phase (SSM, 2016a) are understood to be under active consideration by SKB (SSM, 2016b):
- Detailed narrative of transport across the geosphere-biosphere interface in the key release objects (specifically 157_2 here).
- Investigation of potential transient effects on near-surface hydrology as the climate changes from temperate to periglacial and back to temperate. This is believed to be part of SKB's forward programme.

Outstanding issues
The RFI process has been successful in clarifying the issues identified at the end of the initial review phase. There are four remaining areas of interest to which further attention could be given. Three of these concern potential model review using SSM's dose assessment modelling tool, GEMA-Site, to investigate the importance of the hydrological interpretation in Object 157 (Sections 2.2, 3.3 and 4.1), and the fourth refers to the combination of near-field/far-field sample sets with the biosphere (Section 4.2.1).

Combining probabilistic models with different sized sample spaces
This is something that SKB should be asked to address. The limited modelling carried out in Section 4.2.1 suggests that the combination of datasets with different sample sizes is reasonable for simple models. SKB should be asked to verify, by additional model calculations or other means, that this is also the case for the more complex models combined in SR-PSU.

Alternate modelling of the potential impact of landscape object hydrology
Use of GEMA-Site as an alternate conceptual model is suggested in the investigation of the interpretation of the landscape evolution because it is formulated to be

flexible in respect of the interpretation of evolving hydrology in a way that the SKB models are not.

In particular the issue of the influence of sub-horizontal transport in the soils of Object 157_1 to 157_2 and to the lake in the lower can be readily addressed. However, the radionuclide for which aspect of the model interpretation is most sensitive is ^{14}C. To implement ^{14}C in the current GEMA-Site model would require a review of FEPs specific to ^{14}C in the SR-PSU landscape modelling and their inclusion in the GEMA-Site framework. Interpretation of GEMA-Site for the Object 157 landscape objects would allow alternative calculation of doses for the following cases:

- Migration of radionuclides downslope from the release location in Object 157_1 towards 157_1 soils and lake
- Investigation of the potential for ^{14}C to accumulate in the lake in Object 157_2
- A more comprehensive expression of the processes affecting the leaching of carbonate from Forsmark soils.

A review of the implementation of GEMA-Site to account for releases upslope is recommended as the object in SR-Site that gave the highest doses was on the southern side of the Forsmark pier (opposite to 157_1) and was similarly characterised as an upslope release compared to the default interpretation where input is at the lowest elevation of the basin.

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APPENDIX 1

Requests for further Information – SKB's response

Following the April 2016 meeting, a set of detailed requests for further information were forwarded to SKB. These had been discussed during the meeting. The following is the text of SKB's response. The data provided in the response has been used in the detailed investigations in this main phase report.

Svar till SSM på begäran om förtydligande komplettering av data för konsekvensanalysberäkningar

Strålsäkerhetsmyndigheten, SSM, har till Svensk Kärnbränslehantering AB, SKB, skickat en begäran om komplettering av ansökan om utökad verksamhet vid SFR. Begäran om komplettering som är daterad 2016-07-01 avser data som används inom ramen för konsekvensanalysen i SR-PSU.

SKB översänder härmed begärda data, resultat och beräkningsexempel. Leveransen består av detta brev, tillhörande datafiler och tre PM tillhörande fråga 10 (bilaga 1), fråga 11 (bilaga 2) och fråga 12 (bilaga 3). Följande text förtydligar leveransen för respektive fråga. Beskrivningarna är på engelska eftersom begäran om komplettering var framtagen med hjälp av SSM:s externa experter. Vid behov bistår SKB gärna med ytterligare förtydliganden, förslagsvis genom möten där genomgång av data sker.

The requested material is delivered in a separate folder for each request (fråga#). There are two exceptions to this rule, namely:

- Files associated with request 1 and 2 are delivered in one common folder (fråga1_2).
- Information requested in #5 is provided in folder fråga_8 (as specified below)

1. The 20 m DEM describing land surface, lake bottoms, and lake sediment surfaces (Figure 3-1 of R-12-03). Initial DEM + perturbed DEM as a results of landscape evolution (if possible).

The 20 m DEM is delivered in the folder 'DEM_SR-PSU'.

The perturbed DEM is given in the folder 'Dyn_jorddjupsmodell_GW_SR_PSU', which holds a subfolder for each time step (named -8500AD, -8000AD, … 40 000 AD). The file '[X]ADpdem.asc' (in each subfolder) describes the perturbed DEM for the specified time step X.

2. R-13-22 calculated updates the regolith model at 500 year intervals. To match the documented MIKE-SHE hydrology DEM at 3000, 5000 and 11000

CE the regolith depth model (RDM) results for each layer in the landscape at each of these times should be provided.

The regolith lake development model (RLDM) gives the depth of different regolith layers over time. In the folder Dyn_jorddjupsmodell__GW_SR_PSU, SKB provides files that describes the upper and lower surface for each regolith layers for 500 year time step from -8500 AD to 40 000 AD (in subfolders with the name of the time step). For each time step files are given which represents the upper surface for each layer respectively (Table 1).

Table 1. Files with different regolith layers. [X] denotes the time step.

File name	Regolith type
[X]ADpdem.asc	Organic sediments (peat) (DEM)
[X]ADlpgd.asc	Lacustrine postglacial fine-grained sediments
[X]ADmpgd.asc	Marine postglacial fine-grained sediments
[X]ADgkl.asc	Glacial clay
[X]ADglfl.asc	Glaciofluvial sediment
[X]ADfill.asc	Artificial fill from the RDM
[X]ADtill.asc	Till
[X]ADbedr.asc	Bedrock adjusted for the shoreline displacement, i.e. height coordinate is given relative to the sea level of the time step

3. Biosphere object boundaries as depicted in Appendix 1 of TR-14-06 in GIS format.

The biosphere objects are delivered in GIS format in the file 'BiosfarsObjekt_SR_PSU.shp'.

4. Exit point locations for radionuclides into the biosphere at each of the six "time slices" (as discussed during the meeting). The reference is Figure 4-15 of R-13-25.

The delivery contains trajectory statistics and particle exit locations for 17 bedrock cases and 6 selected time steps.

The data in the folder reflect particles uniformly released in INDIVIDUAL waste vaults of SFR 1 and SFR 3. Trajectory statistics are only calculated inside the bedrock (not inside tunnels, not inside Hydraulic Soil domain (HSD)).

The delivery is organised according to the following file-name convention:
[Bedrock case]_[Extension layout]_[Time step]_[Release location]_[File type].dat

The delivery is further described in the file 'Td11_Exit locations__READ_ME'.

5. Details of release vs. time for all radionuclides and release locations for each of the climate scenarios. N.B. it is likely that these data are included with, or can be calculated from, the Ecolego models and data included in the request below. If this is the case SKB should indicate how to obtain the data for release rates.

Release vs. time for all radionuclides for each of the climate scenarios can be obtained from the Ecolego '.eas'-files for each waste vault. Table 2 lists all required folders in which models for each waste vaults are contained. All except the "Glacial and post-glacial conditions CC" (CCR_GC) use the same release to the biosphere listed as CC1 (also in question 8). For location in the landscape used in the calculations, SKB has assumed that all of the release will discharge in biosphere object 157_2 for all climate scenarios except during the cold period in CCM_EP in which the release is assumed to discharge in either biosphere object 157_1 or biosphere object 114.

Table 2. Folders containing Ecolego '.eas'-files sufficient to extract deterministic (D) and probabilistic (P) radionuclide release vs. time for all radionuclides and waste vaults for each of the climate scenarios.

Folder name	Calculation case	D/P	Original SVN-path (svn://svn.skb.se/kalkyl/SFR/SR-PSU/)
CC1	CCM_GW/CCM_EP/CCR_EX	D	/Indata/NearfieldAndFarfieldModels/
CCP1	CCM_GW/CCM_EP/CCR_EX	P	/Indata/NearfieldAndFarfieldModels/
CC19	CCR_GC	D	/Indata/NearfieldAndFarfieldModels/
CCP19	CCR_GC	P	/Indata/NearfieldAndFarfieldModels/

6. With reference to Figures 4-11 and 4-12 of R-13-25, the following data in GIS format:
Low-magnetic lineaments (black lines in Figs 4-11 and 4-12)
Boundaries of hydraulic domains (grey areas in Figs 4-11, 4-12)

The requested data is provided in the zip-file 'dz lineament.zip'.

'lineament forsmark.shp' contains a shapefile with low magnetic lineaments from Figure 4-11 and 4-12 in report R-13-25.

'forsmark_dz_0m.shp' contains a shapefile with boundaries of hydraulic domains from Figure 4-11 and 4-12 in report R-13-25.

7. The data file that allows the SFR1 and SFR3 repositories to be drawn in GIS format. See, for example, Appendix 1 of TR-14-06.

In the folder 'GIS-delivery Layout SFR' there are files that allows SFR 1 and SFR 3 to be drawn in GIS.

'Layout_SFR1-POS_FR_FJA_12641.shp ' is a shapefile with the layout of SFR 1 (existing repository). The data layer corresponds to the example figure in Appendix 1 TR-14-06. Coordinate system RT90 2.5 g V.

'Layout_SFR3_ver20-SWI_FR_INF_12881.shp' is a shapefile with the layout of SFR 3 (extension). The data layer corresponds to the example figure in Appendix 1 TR-14-06. Coordinate system RT90 2.5 g V.

8. The Ecolego 'EAS' files and associated inputs sufficient to reproduce deterministic and probabilistic results for the main scenario (global warming and early periglacial variants).

Table 3 lists all required files sufficient to reproduce both deterministic and probabilistic results for the main scenario. The Ecolego '.eas'-files are self-propelled with all sufficient input data correctly imported. Since the waste vaults together with attached geosphere models are separate Ecolego-models; the radionuclide discharge needs to be updated in the biosphere and dose-calculation models if any changes have been performed. In SR-PSU this was performed by exporting the radionuclide discharge from each waste vault after simulation to Ecolego '.ear'-files and then imported and the data was linked to discharge variable in the biosphere and dose calculation models. These steps might be cumbersome to do manually, but they are indeed doable. Similar approach has been performed for probabilistic input parameter values since the same set of values was required between different calculation cases.

Table 3: Ecolego '.eas'-files sufficient to reproduce deterministic (D) and probabilistic (P) results for the main scenario; i.e. the global warming (CCM_GW and CCM_TR) and early periglacial (CCM_EP) variants. Files listed represent models for biosphere transport and dose calculations. Folders listed contain near-field/far-field models for each waste vault.

File/Folder name	Calculation case	D/P	Type	Original SVN-path (svn://svn.skb.se/kal-kyl/SFR/SR-PSU/)
LandscapeMainChain_CC1.eas	CCM_GW	D	File	/Simulation/Assessments/
LandscapeMainChain_CCP1.eas	CCM_GW	P	File	/Simulation/Assessments/
LandscapeMainChain_CC6.eas	CCM_TR	D	File	/Simulation/Assessments/
LandscapeMainChain_CCP6.eas	CCM_TR	P	File	/Simulation/Assessments/
LandscapeMainChain_Cold_CC2.eas	CCM_EP	D	File	/Simulation/Assessments/
LandscapeMainChain_Cold_CCP2.eas	CCM_EP	P	File	/Simulation/Assessments/
CC1	CCM_GW/CCM_EP	D	Folder	/Indata/NearfieldAndFarfieldModels/
CCP1	CCM_GW/CCM_EP	P	Folder	/Indata/NearfieldAndFarfieldModels/
CC6	CCM_TR	D	Folder	/Indata/NearfieldAndFarfieldModels/
CCP6	CCM_TR	P	Folder	/Indata/NearfieldAndFarfieldModels/

9. Copies of the following figures from the Biosphere Synthesis Report (TR-14-06) at scale similar to that used in Figure 6-10 of the same report: Figures 3-2, 3-3, 3-4, 4-6, 5-4, 5-6, 5-7, 5-8 and 5-9.

In the three files 'Figures_Chapter_3_TR-14-06', 'Figure_Chapter_4_TR-14-06', and 'Figures_Chapter_5_TR-14-06' the requested figures are presented in a similar scale as the one used in Figure 6-10.

10. Results for a variant calculation that includes drainage of 157_2 into 157_1 via a stream together with an associated commentary.

SKB has answered this request by a PM (Saetre and Ekström 2016) which examines how the assumptions made on the surface water outlet from the main discharge area affects the calculated dose. The variant calculations show that the effects of adding a

stream to the hydrological description of object 157_2 has a marginal effect on the accumulation of radionuclides and on the calculated dose, in the primary discharge area. A redirection of the inlet water to the down-stream object (157_1), from the wetland areas to the open water component of the recipient, will however affect both the accumulation of radionuclides and degassing of C-14 in the down-stream object. In addition, an upper boundary for the concentration of radio carbon in stream and lake water was calculated by allowing the geosphere release to reach a stream directly. None of the variant calculations results in a significantly higher dose than those calculated with the original model, and it is concluded that uncertainties with respect to the presence of a stream in object 157_2, do not have a significant effect on the overall assessment result in SR-PSU.

11. The raw databases used as a basis for the Kd and CR parameterisation.

In SR-PSU parameterisation workflow, two Access databases have been utilised as tools in order to manage the vast number of parameters, samples and data sources. In the first database, SKB_chemistry_SR_PSU.accdb, site-specific K_d and CR values are derived from site-specific concentration measurements and literature data is compiled. In the second database, SKB_Kd_CR.accdb, all available data are compiled and automated functions supports the selection process for each specific parameter case. The implementation of the entire parameterisation process in dynamic databases implicates that there is a traceable link between raw data and the final parameter values.

In addition to the original database files, one document (Grolander and Tröjbom 2016a - Guide to the implementation of the SR-PSU K_d and CR parameterisation in two Access databases) is provided where the implementation of the entire parameterisation process is described. This document assumes that the reader is familiar with both the contents of the report Tröjbom *et al*. 2013 (R-13-01), and Access database programming. The objective with the main part of this document is to illustrate the SR-PSU K_d and CR parameterisation process using three examples that in detail describe the process from beginning to end. The second part of the document is a technical appendix where database objects and code are further described. This latter part was compiled mainly in order to facilitate future updates of the parameterisation, but may also be useful when reviewing the databases and understanding the structures of the databases.

During the review it is recommended that the reader of the document also has access to the three Excel-files listed in Table 4.

Table 4. Files needed for reviewing the databases as described in 'Guide to the implementation of the SR-PSU Kd and CR parameterisation in two Access databases'

File name	Description
SKB_chemistry_SR_PSU.accdb	Access database where site specific K_d and CR values are derived
SKB_Kd_CR.accdb	Access database that compiles all available data and implements the data selection process
Coupling parameters to data_ver3.xlsx	Interface Excel-file where each parameter is coupled to appropriate site data.
ParamClass.xlsx	Interface Excel-file where parameters are associated to specific site data and literature data sources. Sources are also ranked in this table.
FinalTable_cond_fix_PLOTB.xlsx	Excel-file containing figures where Kd and CR are compared for elements across parameters. This supporting information is not included into the report.

12. Worked examples of the derivation of Kd and CR for the following radionuclides (identified as being important in the initial review of biosphere modelling for specific radionuclides): Ca-41, Ni-59, Mo-93, I-129, U-238

In the SR-PSU assessment for the biosphere, K_d parameters were derived for nine soils and particulate matter, 55 CR parameters were derived for terrestrial, limnic and marine biota and two transfer factors were derived for cow milk and meat. This gives in total 69 parameters and for each parameter 31 elements were parameterised, which sums up to 2,139 unique parameter cases handled. Worked examples for the five listed nuclides for all K_d and CR parameters correspond to 330 unique cases.

The parameters were not manually derived but automated functions in the Access database `SKB_Kd_CR.accdb` were used to achieve K_d and CR values. Nevertheless, manual reproduction of the parameters is doable. The document (Grolander and Tröjbom 2016b -Manual reproduction of parameter values) includes worked examples for two parameters (one K_d and one CR parameter) for the five requested nuclides. The examples in this document can be seen as instructions on how to manually reproduce and review any parameter case of interest based on the original data files provided and the information on data selections given in Tröjbom et al. 2013. This can be seen as one option to review and quality assure the K_d and CR data selection process and the resulting parameter values without the need to investigate the database tools in detail.

Files needed for manually reproduce and review the selected parameter values are listed below (Table 5).

Table 5. Files needed for manually reproduce and reviewing the databases as described in Manual reproduction of parameter values'

File name	Description
Matched_SNO.xlsx	Excel-file that specifies which sample pairs are combined for the calculation of K_d and CR.
SKB_Chemistry_SR_PSU.xlsx	Excel-file with site specific concentrations data.
Kd_CR.xls	Excel-file that compiles all available site-specific data and literature data.
ConversionFactors.xlxs	Excel-file with conversion factors derived from IAEA data on carbon and dry matter content.
Excluded_sampels.xlsx	Excel-file that lists site-specific samples excluded during the parameterisation process.
DMC & CC database.xlsx	Excel file that contains dry matter and carbon content data from IAEA.

Med vänlig hälsning

Svensk Kärnbränslehantering AB
Projekt SFR Utbyggnad

Peter Larsson
Projektledare

Bilagor

1. *Saetre P, Ekström P-A, 2016. Drainage of runoff water from 157_2 into157_1 via a stream – Biosphere complementary information for SR-PSU,* SKBdoc 1554499, ver 1.0, Svensk Kärnbränslehantering AB
2. *Grolander S, Tröjbom M, 2016a. Guide to the SR-PSU parameterisation of Kd and CR*, SKBdoc 1555970, ver 1.0, Svensk Kärnbränslehantering AB
3. *Grolander S, Tröjbom M, 2016b. Manual reproduction of parameter values*, SKBdoc 1556279, ver 1.0, Svensk Kärnbränslehantering AB

Alla dokument och datafiler levereras till SSM på ett usb-minne. Dokumenten och datafilerna finns lagrade hos SKB på följande plats: svn.skb.se/trac/PSU/browser/Tillståndsansökan/Komplettering_aug_2016

2

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In-depth review of key issues regarding biosphere models for specific radionuclides in SR-PSU

Activity number: 3030014-1019
Registration number: SSM2016-3262
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Abstract

SKB has submitted an application to SSM for expansion of the final repository for low and intermediate level radioactive waste at Forsmark (SFR). SSM has contracted a number of organisations to support its review of SKB's safety analysis (SR-PSU), with each organisation contributing to the review of a different technical area. SSM has divided its review activities into an initial review phase and a main review phase. This report describes the findings of Quintessa Limited's main phase review of the analysis of biosphere modelling for specific radionuclides in SR-PSU.

The SR-PSU assessment adopts a complicated approach to representing potential contamination of the biosphere and its radiological significance over a time scale of tens of thousands of years. SR-PSU represents a further iteration on previous assessments for the SFR facility. Iteration and the proximity of some of the calculated results to the risk criteria provide drivers for some of the complexity in the modelling approach, along with interpretation of the significant amount of information derived from characterisation of the present-day biosphere.

The large uncertainties inherent in projecting potential consequences of radioactive waste disposal over extremely long periods mean that assessment results can only be taken as broad indicators of environmental safety and are typically based on conservative assumptions with regards to potential exposure. The degree of complexity in the biosphere modelling approach, together with a combination of assumptions with regards to radionuclide releases to the biosphere and potential exposures, mean that conservatisms have been removed in relation to previous assessments.

The principal conclusions from the main review phase for the SR-PSU assessment with regards to biosphere modelling for specific radionuclides are summarised below. These findings are drawn from three review activities, which were prioritised based on an initial review phase:

- independent implementation of the SR-PSU biosphere models with a view to verifying results and gaining a thorough understanding of the modelling approach adopted;
- in-depth review of the modelling of C-14; and
- detailed review of the derivation of parameter distributions for sorption coefficients (K_d) and concentration ratios (CR).

The findings should be read in conjunction with the findings of the initial review phase.

The main conclusions drawn from independently implementing the SR-PSU biosphere model are summarised below.

- The biosphere mode is extremely complicated, requiring 280 equations in the Biosphere Model Report, and 56 compartments/158 transfers in a cut-down implementation. Nonetheless, the model and data are comprehensively documented and have permitted the results to be largely reproduced (to within about a factor of two).
- The modelling approach represents a hybrid between a probabilistic and deterministic model, in which PDFs are assigned to a very large number of biosphere parameters while key aspects of the modelling are represented deterministically. The distribution of results from probabilistic calculations is therefore an incomplete measure of parameter uncertainty.

- The Ecolego modelling makes use of deterministic 'hard-wired' values for some key parameters, including peat thickness and scaling factors used for agricultural soil concentrations, in a way that makes the values used inconsistent with underlying parameters in probabilistic calculations.
- Simplifying assumptions exacerbate the rapid rate of loss of C-14 to the atmosphere, notably the neglecting of horizontal water flows in sub-surface layers in the terrestrial modelling.
- The Ecolego implementation was found to differ from the model specification in calculating the radionuclide concentrations in drained mire soils in a way that reduces the associated results by about a factor of five (i.e., if SKB's model specification is correct, then the SR-PSU results for the drained mire farmer should be about a factor of five higher).
- Human habit assumptions result in a relatively low degree of exposure for some of the exposure groups, notably:
  - very low capture fractions for drilled wells.
  - the drained mire and garden plot groups spend only 54 hours per year on contaminated soils;
  - the garden plot group obtains only 8% of their dietary carbon from the goods that they produce;
  - the larger hunter-gatherer group is the only one that consumes fish, which was a key exposure pathway in previous assessments;
  - the equivalent of 30 adult individuals used as a basis for the hunter-gatherer group effectively dilutes exposure in comparison to other groups such that only 0.7% of dietary intake comes from the most contaminated biosphere object after terrestrialisation.
- Explicit dynamic modelling of agricultural soil concentrations was able to reproduce the results of the analytical approach adopted in SR-PSU for drained mire soils with the exception of relatively short-lived radionuclides, for which the analytical approach was found to underestimate concentrations.

The main conclusions drawn from review of the SR-PSU biosphere model for C-14 are summarised below.

<u>Conclusions regarding the regolith:</u>

- Organic carbon pools have been explicitly introduced to improve the way that the carbon balance is represented.
- The existence and distinction in the behaviour of $^{14}CH_4$ in regolith layers, notably in the mire, is not discussed at all and is completely neglected in the biosphere modelling.

<u>Conclusions regarding the aquatic ecosystem:</u>

- The assumed release to biosphere object 157_2, which does not have a water body, means that people are less exposed to contaminated fish (much of the C-14 degasses from the mire surface before reaching the lake that is present in Object 157-1), the consumption of which dominated the C-14 dose in the SAR-08 assessment.
- The modelling approach adopted for C-14 accumulation in fish results in significantly lower concentration ratios when compared against IAEA recommended values.

<u>Conclusions regarding the terrestrial ecosystem:</u>

- The assumed degassing rates from soil are much higher than those used in other assessments. There is potential for further comparison of the rates against more recent literature sources.
- The assumed refractory organic matter content is lower than might be expected for mire vegetation such as *Spaghnum* moss. This leads to a

greater proportion of decayed matter entering the soil pore water, for release to the atmosphere, than might be appropriate for such ecosystems

Conclusions regarding the atmospheric sub-model:

- The new atmospheric exchange model provides an improved representation of micrometeorological processes. Similar models have been adopted by other waste management organisations in support of their safety assessments over recent years.

The main conclusions from in-depth review of the derivation of K_d and CR values for the SR-PSU assessment are summarised below.

- The highly automated process(es) of extracting site-specific data from SKB's data archives, and using these to calculate and 'quality assure' K_d and CR values, is complex but ultimately traceable with the aid of the additional explanatory documents provided by SKB.
- This traceability is less obvious when reading the original K_d and CR Report.
- Even given the explanation of the automated data handling processes, the complexity of these procedures may lead to a loss of focus on the importance of the parameter values produced. The eventual statistical power of the site-specific parameters obtained is limited by low numbers of data pairs from which K_ds and CRs can ultimately be calculated (e.g. N=7 for K_d RegoLow for nickel; N=1 for CR for nickel in fish; N ranges from 1 to 11 for Mo and Ni K_d values across all soil & sediment types).
- Several methods have been applied to compensate for this lack of statistical power, including the use of the statistical variation of ALL elements to represent plausible variation in a parameter for a single element. This approach seems arbitrary and may reflect a pragmatic need to increase the apparent statistical power of the data analysis in the face of very low numbers of site-specific parameter values available to SKB.
- SKB concedes that the process of defining the plausible limits of CRs and K_ds is "*to some extent subjective and based on the general assumption that it is conservative to widen the PDFs of selected parameter data*" based on the use of GSDs for all elements.
- A more richly-replicated site-specific database (i.e. more and better-targeted measurements at Forsmark and Laxemar-Simpevarp) would have circumvented the need for such complex and debatable statistical approaches. It would also have reduced the reliance on and influence of the authoritative but ultimately limited literature sources incorporated within the SR-PSU assessment.

Contents

1. Introduction

SKB has submitted an application to SSM for expansion of the final repository for low and intermediate level radioactive waste at Forsmark (SFR). SSM has contracted a number of organisations to support its review of SKB's long-term safety analysis (SR-PSU), with each organisation contributing to the review of a different technical area. SSM has divided its review activities into an initial review phase and an in-depth review of key issues for the main review phase.

Findings of the initial review phase for biosphere modelling in SR-PSU are described in SSM (2016). This report describes the findings of the main phase of Quintessa Limited's review of the analysis of biosphere modelling for specific radionuclides in SR-PSU. In the context of this report, 'specific radionuclides' means radionuclides that are important to the consequence analysis of potential releases from the SFR.

The main phase review of biosphere modelling for specific radionuclides in SR-PSU covered three main components.

- SKB's biosphere models were independently implemented in a different software tool; the associated findings are described in Section 2.
- An in-depth review of SKB's model for C-14 in the biosphere is described in Section 3.
- A detailed review of SKB's approach to deriving equilibrium sorption coefficients (K_ds) and biosphere concentration ratios (CRs) is described in Section 4.

Overall conclusions are summarised in Section 5.

At the time of SKB's submission to SSM, the supporting documentation that describes the approach taken to the representation of the biosphere in the SR-PSU assessment was incomplete. Since the completion of the initial review phase, two reports that were not available during the initial review phase have since been published and have therefore been encompassed in the main review phase:

- The Biosphere FEP Handling Report: R-14-02, which was published in November 2015 (SKB, 2015).
- The Atmosphere Model for C-14: R-15-09, which was published in November 2016 (Avila and Kovalets, 2016).

This report also refers to the following SR-PSU reports:

- The Main Report: TR-14-01 (SKB, 2014a);
- The Radionuclide Transport Report: TR-14-09 (SKB, 2014b);
- The Biosphere Synthesis Report: TR-14-06 (2014c);
- The Biosphere Model Report: R-13-46 (Saetre et al., 2013);
- The Biosphere Parameter Report: R-13-18 (Grolander, 2013);
- The K_d and CR Report: R-13-01 (Tröjbom et al., 2013); and
- The Biosphere FEP Report: R-13-43 (SKB, 2013).

2. Independent Implementation of the SR-PSU Biosphere Model

The biosphere model for the SR-PSU assessment is complex and is described in the Biosphere Model Report with over 280 equations. The large amount of input data required by the model is described in the Biosphere Parameter Report and the K_d and CR Report. A compartment modelling approach is adopted for assessing the biosphere, whereby the time-dependent amounts of radionuclides in each compartment are calculated based on releases into the biosphere from the geosphere, transfer rates around the biosphere, losses from the biosphere region of interest and accounting for radioactive decay and in-growth.

The model is implemented by SKB in the Ecolego modelling software. As part of the review process, the model has been independently implemented in a different compartment modelling software tool with the objectives of:

- reviewing the completeness of the model specification;
- verifying the results presented by SKB; and
- developing a greater insight into the complex SR-PSU biosphere model.

The compartment modelling software tool used for the independent implementation of the SR-PSU biosphere model is the AMBER software (Quintessa, 2016a). AMBER is an established compartment modelling tool with a track record of application to safety assessments for radioactive waste disposal (Quintessa, 2016b). The software is developed and maintained within an accredited software quality assurance programme and is used as a benchmark against which Ecolego has previously been tested (Maul et al., 2003, 2004; Walke et al., 2015).

The findings of the independent implementation of the SR-PSU biosphere model are reported in this section.

- A summary of the model's implementation in AMBER is provided in Section 2.1.
- Results of the AMBER implementation are compared against the Ecolego results in Section 2.2.
- Observations about the SR-PSU models are reported in Section 2.3.

2.1. Implementation in AMBER

The compartmental structure of the AMBER implementation is described in Section 2.1.1. The interpretation of the input data is described in Section 2.1.2. The implementation of the biosphere transfer processes is described in Section 2.1.3. The exposure calculations are described in Section 2.1.4.

The implementation has focused on the *global warming variant* of the main SR-PSU scenario; the other variant to the main scenario, the *early periglacial variant*, does not result in higher calculated doses.

The comparison has been aided by SKB's provision of the Ecolego calculation files used in its assessment. Any information not clearly documented in the SR-PSU reports that required investigation of the underpinning Ecolego files is highlighted.

2.1.1. Compartmental Structure

The AMBER implementation focuses on representing the part of the surface environment ("biosphere object") that receives 100% of the geosphere discharge in the main SR-PSU assessment calculations (Object 157-2) together with its two down-stream objects (Objects 157-1 and 116). Each biosphere object has the same compartmental structure, illustrated in Figure 1, which includes both aquatic and terrestrial components.

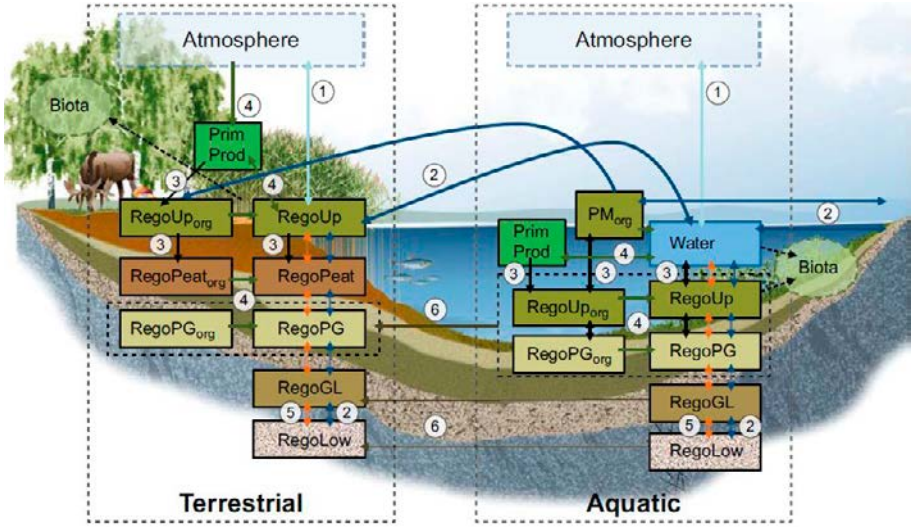

Figure 1: Discretisation of the SR-PSU model for each biosphere object[1] (Figure 3-1 of the Biosphere Model Report, which includes definitions for the numbered processes and coloured arrows).

Within the AMBER implementation, each set of object compartments is organised within a sub-model. The top-level AMBER model is shown in Figure 2. Marine transfers out of these objects were directed to a single compartment representing other parts of the Öregrundsgrepen ('Grepen' in Figure 2). Transfers out of the region of interest are directed to a 'Sink' compartment.

[1] "Rego" refers to regolith layers; PG refers to post-glacial deposits; GL refers to glacial clay; the subscript "org" refers to organic matter; PM refers to particulate matter; and "Prim Prod" refers to primary producers (plants and algae).

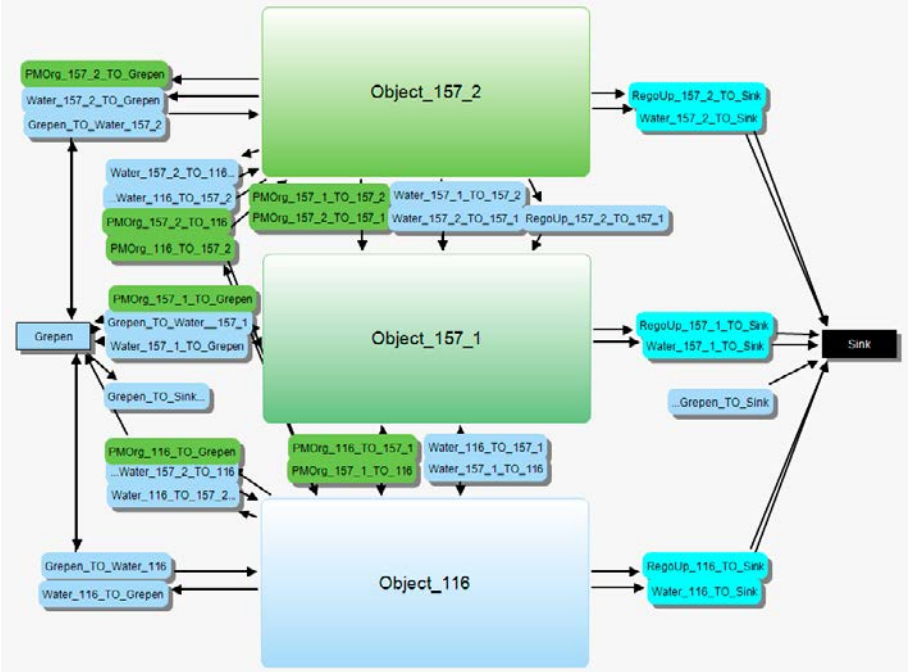

Figure 2: Top-level structure of the AMBER compartmental model. Compartments are rectangular with black borders. Rounded labels with arrows indicate transfer between compartments. Graded rectangles indicate sub-models that contain other compartments. Note that the groundwater source terms into the biosphere are not illustrated in this figure because they are contained within the sub-models (see the red boxes in Figure 3).

The compartmental structure adopted for each biosphere object is shown for Object 157-2 in Figure 3. Note that there are some pragmatic simplifications in comparison to the Ecolego model, most notably:

- only a single compartment is used for the aquatic primary producers, compared to three separate compartments in Ecolego (the additional complexity is expected to be of negligible benefit); and
- the atmosphere is not explicitly represented with compartments (uptake by plants are air concentrations are defined in the SR-PSU model based on the release flux from the soil).

A total of 56 compartments and 158 transfers are needed to represent the SR-PSU biosphere model for Objects 157-2, 157-1 and 116.

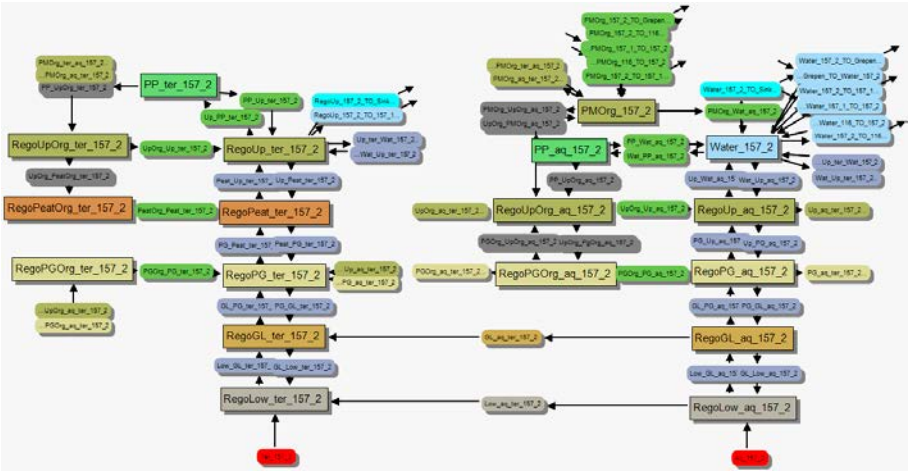

Figure 3: Compartment structure for biosphere Object 157-2, reflecting the structure illustrated in Figure 1. Red boxes indicate external radionuclide source-terms to the biosphere. The same structure is used for biosphere Objects 157-1 and 116.

2.1.2. Input Data

Contaminants and Decays
The Biosphere Synthesis Report presents deterministic results for unit releases of radionuclides in groundwater to Object 157-2; the total doses for unit release calculations are termed Landscape Dose Factors (LDFs) by SKB. The AMBER implementation has been set-up to track the radioactive decay of each radionuclide entering the biosphere, so that LDFs can easily be calculated for unit releases. This means that some isotopes are included more than once, as they relate to different decay chains. Consequently, there are 151 contaminants used to represent the 55 radionuclides included in the model and 156 associated radioactive decays (there are more decays than contaminants due to the branching of the Am-242, Cm-243 and Pu-241 decay chains). So, for example, there are nine types of Ra-226 being modelled, explicitly distinguishing that in-grown from Th-230, U-234, U-238, Pu-238, Pu-242, Am-242, Cm-242 and Cm-246 entering the biosphere, as well as the Ra-226 entering the biosphere itself.

Time-dependent Inputs
Biosphere objects within the SR-PSU model can evolve with time due to post-glacial up-lift, resulting an areas transitioning from marine to terrestrial systems. The progression of this transition is parameterised based on supporting landscape evolution modelling and is reflected in the Ecolego model with time-dependent parameters and transfer processes. The Biosphere Parameter Report gives the time-dependent values for input parameters in Appendix C (biosphere object data) and Appendix D (hydrological data). This data is drawn directly into the AMBER implementation via text-based import files.

In addition to the biosphere object properties and water exchanges, a time-dependent deterministic groundwater source-term from the geosphere to the biosphere for the global warming calculation case (CC1) is also imported into AMBER.

Sampled Parameters
SKB has adopted both deterministic and probabilistic approaches for the SR-PSU assessment. This means that many input parameters are defined with a best estimate

value (for use in deterministic calculations) and a probability density function (PDF) for probabilistic calculations. The AMBER model that encompasses biosphere Objects 157-2, 157-1 and 116 includes 163 sampled parameters. Some of the sampled parameters, such K_d and CR, are indexed over the 33 chemical elements included in the model. Given that each element has its own specific distribution in each of these parameters, it means that the model includes a total of 942 individual PDFs.

PDFs are widely assigned, including, for example a distribution for the width of a barley leaf.

Non-time-dependent Non-sampled Parameters
In addition to the time-dependent parameters, the SR-PSU biosphere model includes nearly 50 biosphere parameters that are not sampled; these are listed in Table 1.

The SR-PSU documentation lacks a discussion of the logic and justification for choosing probabilistic or deterministic representations of specific parameters. Table 1 serves to highlight that:

- landscape evolution and exposure group related assumptions are treated deterministically; and
- there are deterministic parameters for other aspects of the model that are typically treated probabilistically.

Table 1: List of non-sampled biosphere parameters.

Group	Parameters
Landscape evolution parameters	Maximum area of aquatic sediments represented (area_obj), m^2
	Time thresholds related to landscape development (threshold…) y
	Thickness of glacial clay in each object (z_regoGL), m
	Thickness of lower regolith in each object (z_regoLow), m
	Thickness of upper regolith in lakes (z_regoUpLake), m
	Thickness of upper regolith in lakes (z_regoUp_sea), m
Exposure group parameters	Number of individuals in each exposure group (N_group)
	Area of arable land per person (area), m^2 per person
	Total area of land needed to support each individual (area_support), m^2 per person
	Demand for algal fertiliser (demand_algFertil), kgC m^{-2} y^{-1}
	Demand for hay (demand_hay) kgC m^{-2} y^{-1}
	Demand for peat (demand_peat) kg per person
	Dose coefficients (doseCoeff…)
	Fraction of arable area used for each crop (f_area_crop)
	Dietary fractions (f_diet)
	Maximum fraction of fish in diet (f_diet_fish_max)
	Fraction of livestock diet supplied by hay (f_meadow)
	Fraction of inland/outfield farmer's time spent growing crops (f_time_agri)
	Fraction of inland/outfield farmer's time spent growing hay on wet meadows (f_time_hay)
	Consumption rate of peat fuel (fuel_cons_peat), kg y^{-1}
	Consumption rate of peat fuel (fuel_cons_wood), kg y^{-1}
	Ingestion rate of carbon (ingRateC), kgC y^{-1}
	Ingestion rate of water (ingRate_water) L day^{-1}
	Inhalation rate (inhRate) m^3 hr^{-1}
	Duration of external exposure (time_exposure), hr y^{-1}

Group	Parameters
Atmosphere parameters	Height of atmosphere layers (height…), m
	Height of the displacement plane (height_displ)
	Von Karman constant (karman)
	Drag coefficient (dragCoef)
	Surface roughness length (z_0)
Other Parameters	Diffusivity in free solution (D_water), $m^2\ y^{-1}$
	Scaling factors for agricultural soils
	Equilibrium time for peat (t_peat_equilib) y
	Drainage depth for mire agriculture (z_drain_agri), m
	Carbon content of stem wood (f_C_wood)
	Well capture fractions (f_well)
	Water extraction from a drilled well (q_well), L day^{-1}

2.1.3. Biosphere Transfer Processes

To be able to model the evolving amounts of contaminants in compartments, AMBER needs transfer processes between compartments to be defined in terms of rate coefficients (y^{-1}).

The SR-PSU specification is unusual in that the equations for calculating transfers within the biosphere model are defined as transfer rates (Bq y^{-1}) relating to activity concentrations (AC) in the compartments. In addition, the activity concentrations used to specify transfer rates are differentiated between activity concentrations in the dissolved phase (Bq L^{-1}), total volumetric concentrations (Bq m^{-3}), activity concentrations by organic carbon (Bq kgC^{-1}) and activity concentrations by dry mass (Bq kg^{-1}).

Although the notation adopted in the Biosphere Model Report complicated the presentation of the mathematical model, it was found to be comprehensively described. The use of figures summarising the transfer processes for each component of the model was also found to be helpful in interpreting what was described in the text.

2.1.4. Exposure Calculations

The AMBER implementation focuses on reproducing calculations for potential doses to humans; the non-human biota calculations have not been replicated. The AMBER implementation includes the equilibrium models for calculating radionuclide concentrations in agricultural soils.

2.2. Comparison of Results

Comparisons have been made between the results calculated with the AMBER implementation and those calculated with Ecolego with (i) the deterministic CC1 radionuclide fluxes to Object 157-2, and (ii) for unit releases to Object 157-2. These comparisons are described in the sub-sections below.

2.2.1. Comparisons for the Global Warming Case (CC1)

The radionuclide amounts in the upper regolith compartment of Object 157-2 calculated in AMBER and Ecolego with the deterministic CC1 source to the biosphere are compared in Figure 4. The figure shows that the AMBER implementation agrees with the Ecolego results with a factor of about two. This represents a reasonable degree of agreement, given the complexity of the model. The comparison could almost certainly be improved with more detailed investigation, though this degree of agreement is considered adequate for the purposes of the review exercise. The figure highlights the importance of Mo-93 and Ni-59 to the long-term inventories in the inorganic component of mire soils. The dynamics seen the figure reflect a combination of the time-dependent radionuclide releases to the biosphere and the biosphere transitions.

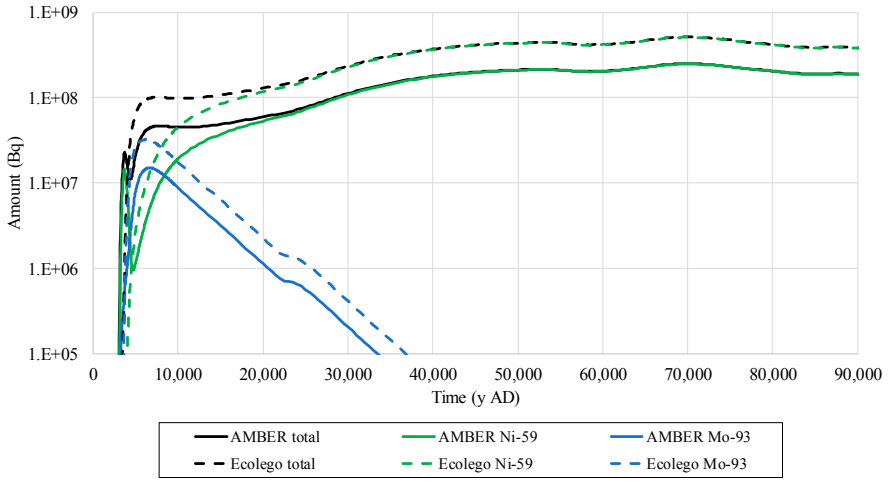

Figure 4: Calculated amounts in the terrestrial inorganic upper regolith compartment of biosphere Object 157-2.

A similar comparison is made for the organic upper regolith compartments in Figure 5. This again shows agreement to within an approximate factor of two. In this case, the figure highlights the importance of C-14 to the inventory in the organic component of mire soils.

The two sets of comparisons for the radionuclide inventory in the upper regolith give confidence that the AMBER model is adequately reproducing the main properties and transfer processes within Object 157-2.

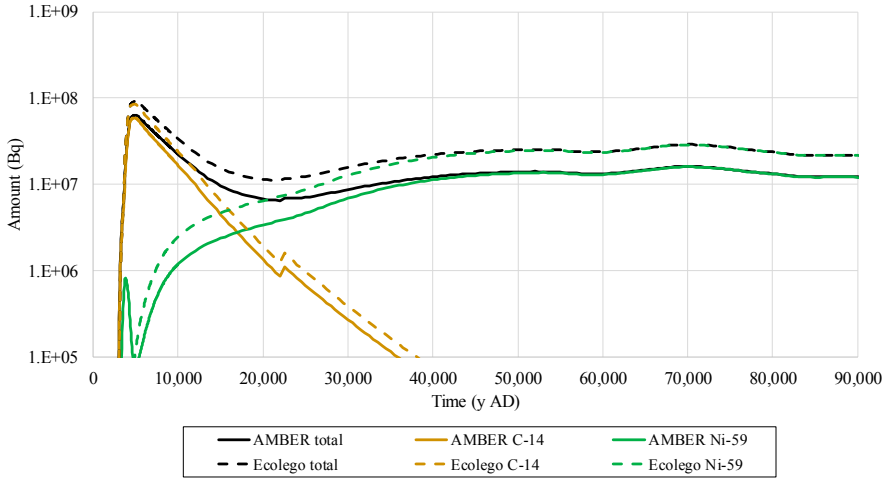

Figure 5: Calculated amounts in the terrestrial organic upper regolith compartment of biosphere Object 157-2.

The calculated concentrations in the terrestrial primary producers in Object 157-2 are compared in Figure 6. As with the soil inorganic and organic inventories, the figure shows agreement to within a factor of about two. The figure also highlights the importance of C-14 and Ni-59 to the activity concentrations in terrestrial primary producers.

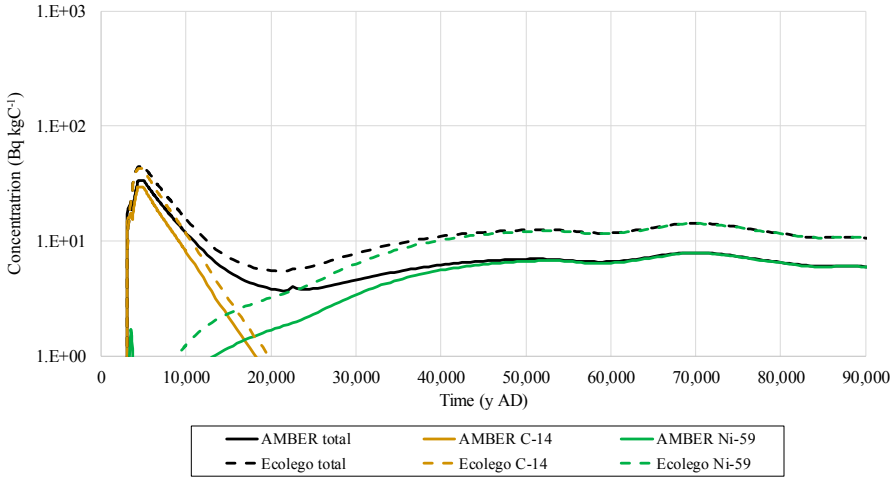

Figure 6: Calculated concentrations in terrestrial primary producers in biosphere Object 157-2.

The total calculated doses for each of the exposure groups is compared in Figure 7. The results for the hunter/gatherer group and the infield/outland farmer agree within a factor of about two. The results are now higher in AMBER by up to about a factor of two for the drained mire farmer and about a factor of three to four for the garden plot group. The results for the drained mire farmer are explored in more detail below.

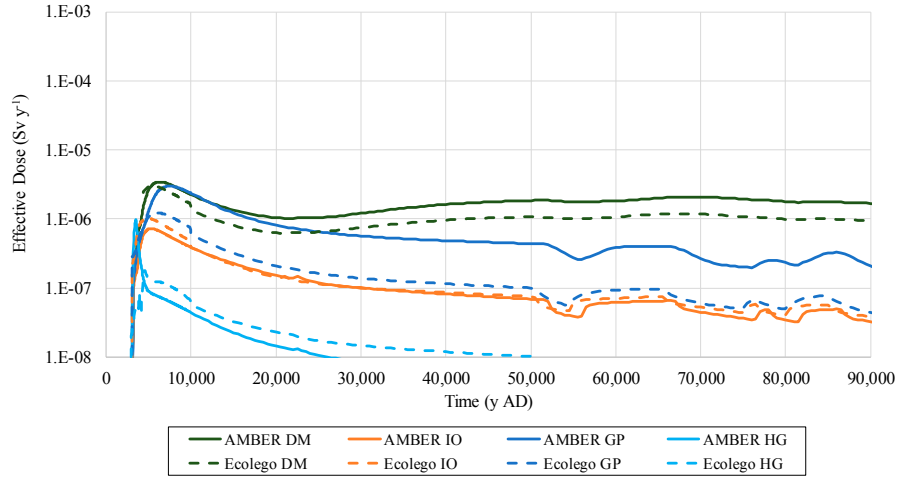

Figure 7: Total calculated effective doses for each of the exposure groups in biosphere Object 157-2. DM = drained mire farmer, IO = infield-outland farmer, GP = garden plot group, HG = hunters and gatherers.

The total calculated effective dose to the drained mire farmer by radionuclide is compared in Figure 8, with the main contributing radionuclides highlighted.

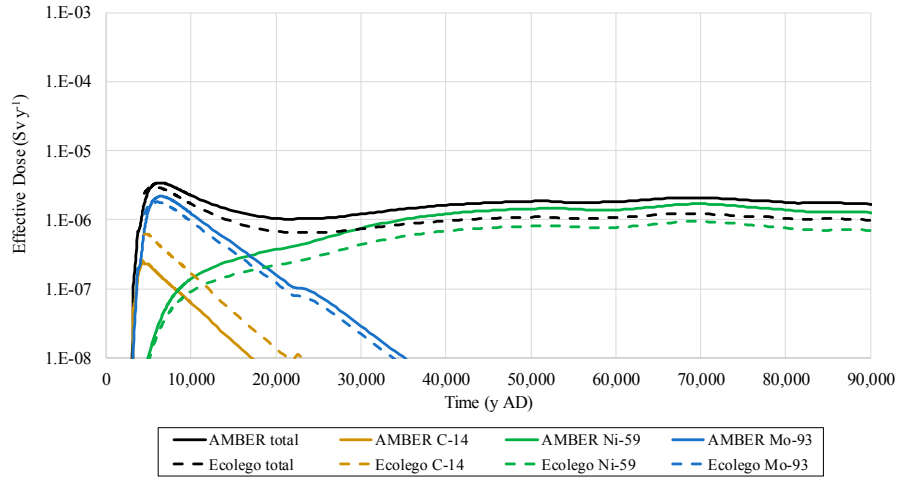

Figure 8: Total calculated effective dose to the drained mire farmer in biosphere Object 157-2.

The calculated effective doses by exposure pathway are compared in Figure 9. This figure shows that ingestion of food dominates and that the AMBER results for ingestion of food are up to about a factor of two higher than those calculated by Ecolego.

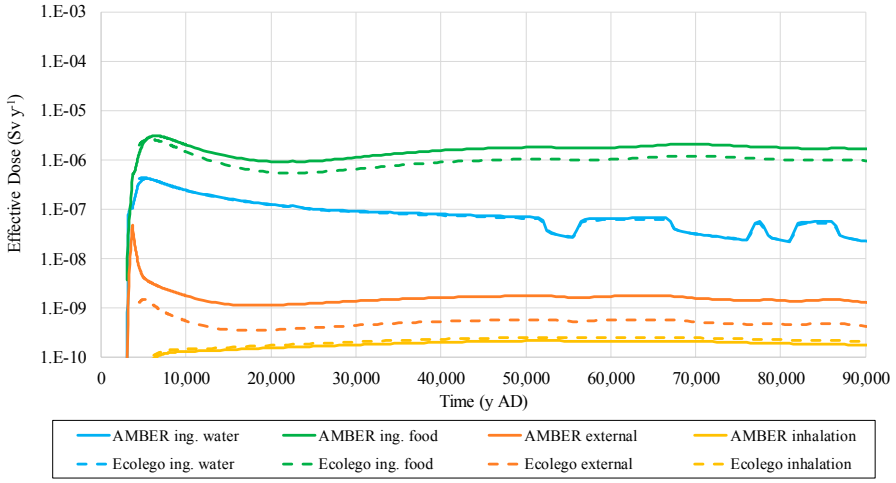

Figure 9: Calculated effective dose to the drained mire farmer in biosphere Object 157-2 by exposure pathway.

Figure 9 also shows that the AMBER results for the drinking water pathway are almost identical to those calculated with Ecolego for the drained mire farmer in Object 157-2. The drinking water for the drained mire farmer in this case is drawn from a dug well, which has higher concentration in comparison to the drilled well. The agreement between the two sets of results reflects agreement in the calculated concentration in groundwater within the terrestrial lower regolith compartment of Object 157-2.

The activity concentrations in drained mire soils are dominated by the contribution from the inorganic soil. Figure 10 compares the AMBER and Ecolego calculated inorganic soil concentrations for the drained mire cereals and shows that the discrepancy in the drained mire dose calculations is due to a discrepancy in the calculation of drained mire soil concentrations. The soil concentration in the AMBER model is based on Equation 7-45 of the Biosphere Model Report. It is noted that the inventory in the drained mire soil is divided by a function including:

$$area_{DM}\, f_{area,i}\, N_{group,DM} \qquad (1)$$

This function gives the area used for each crop. For cereals grown on drained mire in Object 157-2, this equates to 6200 x 0.48 x 10 = 27,760 m^2.

In the Ecolego implementation, the associated parameter ($AC\_RegoUp_{lobj157\_2.doses.Drained\_mire.crop}$) is not divided by the area used for each crop, but is instead divided by the total terrestrial area of Object 157-2, which equates to 147,000 m^2 after 4275 AD. This accounts for a difference of about a factor of five between the results and explains why the lower compartment amounts calculated in AMBER (see Figure 4) become higher concentrations in the agricultural soils.

The inventory in the drained mire soils ($RegoUp_{i,aver,DM}$) already explicitly takes into account the fraction of the mire area that is needed for drained mire agriculture (see the f_{area} parameter in Equation 7-26 of the Biosphere Model Report). Therefore, Equation 7-45 of the Biosphere Model Report is correct to use the drained mire area in the denominator and it would seem that there is an error in the Ecolego implementation.

In reviewing the discrepancy, the comparison was not helped by the numerator in the Ecolego parameter AC_RegoUp$_{lobj157_2.doses.Drained_mire.crop}$ not matching the specification in Equation 7-44 of the Biosphere Model Report (notably $f_{regoUp,aver}$ differs).

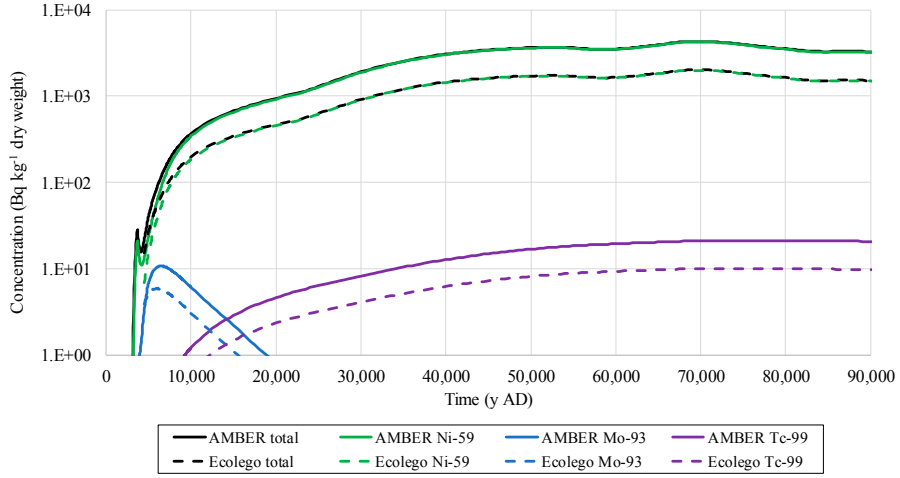

Figure 10: Inorganic component of the radionuclide concentrations in drained mire soil for Object 157-2.

2.2.2. Comparison for Unit Releases

Calculation of equilibrium biosphere dose factors for unit releases to biosphere Object 157-2 (LDFs) provides an additional route for comparing the results of the AMBER implementation against the Ecolego model. Comparing LDFs allows the models for all radionuclides to be compared, rather than just those that are key to the calculated doses. Table 2 presents a comparison between the LDFs in Table 10-1 of the Biosphere Synthesis Report against the highest values between the different exposure groups in the AMBER implementation with a unit release to Object 157-2. The comparison shows good agreement (within a factor of two) for 38 out of the 54 radionuclides compared. Notable differences (AMBER results are more than a factor of ten higher) are observed for Th-230 and U-235.

Consistent with the LDF values given in the Biosphere Synthesis Report, the AMBER values presented in Table 2 are generated for 18,000 AD. It is noted that the LDF values have not reached equilibrium by this time for many of the radionuclides.

Table 2: Comparison of LDFs (Sv y^{-1} per Bq y^{-1}) calculated at 18,000 AD with AMBER against those reported in the SR-PSU assessment.

Radionuclide	SR-PSU	AMBER	Ratio AMBER:SR-PSU
Ac-227	1.0E-11	1.0E-11	1.0
Ag-108m	5.4E-14	3.4E-14	0.6
Am-241	1.7E-12	1.7E-12	1.0
Am-242m	1.6E-12	1.7E-12	1.0
Am-243	2.0E-12	2.2E-12	1.1
Ba-133	1.3E-14	1.3E-14	1.0
C-14	7.9E-15	3.3E-15	0.4

Radionuclide	SR-PSU	AMBER	Ratio AMBER:SR-PSU
Ca-41	6.2E-14	6.3E-14	1.0
Cd-113m	2.2E-13	2.0E-13	0.9
Cl-36	7.5E-13	3.7E-12	4.9
Cm-242	1.0E-13	1.1E-13	1.1
Cm-243	1.3E-12	1.3E-12	1.0
Cm-244	1.0E-12	1.0E-12	1.0
Cm-245	2.2E-12	2.7E-12	1.2
Cm-246	2.0E-12	2.1E-12	1.0
Co-60	3.0E-14	3.0E-14	1.0
Cs-135	2.0E-13	8.1E-14	0.4
Cs-137	1.3E-13	1.2E-13	0.9
Eu-152	1.2E-14	1.2E-14	1.0
H-3	1.2E-15	4.0E-16	0.3
Ho-166m	2.1E-14	3.8E-14	1.8
I-129	8.0E-12	5.9E-12	0.7
Mo-93	5.5E-12	6.0E-12	1.1
Nb-93m	1.0E-15	1.0E-15	1.0
Nb-94	3.8E-14	1.4E-13	3.6
Ni-59	2.9E-14	1.1E-14	0.4
Ni-63	1.7E-15	1.6E-15	1.0
Np-237	1.3E-12	1.8E-12	1.3
Pa-231	8.4E-12	1.1E-11	1.3
Pb-210	6.1E-12	6.2E-12	1.0
Pd-107	1.9E-14	6.8E-15	0.4
Po-210	1.0E-11	1.0E-11	1.0
Pu-238	2.0E-12	2.0E-12	1.0
Pu-239	2.7E-12	2.5E-12	0.9
Pu-240	2.4E-12	2.4E-12	1.0
Pu-241	4.2E-14	4.4E-14	1.0
Pu-242	2.8E-12	2.4E-12	0.9
Ra-226	4.3E-12	1.3E-11	3.1
Ra-228	6.0E-12	6.0E-12	1.0
Se-79	3.0E-13	2.6E-13	0.9
Sm-151	8.5E-16	8.5E-16	1.0
Sn-126	2.0E-13	1.4E-13	0.7
Sr-90	2.8E-13	2.8E-13	1.0
Tc-99	1.7E-13	3.6E-14	0.2
Th-228	1.2E-12	1.2E-12	1.0
Th-229	5.9E-12	6.0E-12	1.0
Th-230	2.4E-12	2.5E-11	10.5
Th-232	2.6E-12	5.6E-12	2.2
U-232	3.0E-12	3.2E-12	1.1

Radionuclide	SR-PSU	AMBER	Ratio AMBER:SR-PSU
U-234	5.7E-12	2.7E-11	4.8
U-235	5.7E-12	6.1E-11	10.7
U-236	5.5E-12	2.5E-11	4.5
U-238	5.4E-12	2.3E-11	4.3
Zr-93	1.8E-13	5.8E-14	0.3

2.3. Conclusions from Independent Implementation

Some overall conclusions can be drawn from the exercise of independently implementing the SR-PSU biosphere models in different compartment modelling software.

The biosphere model is extremely complicated, requiring 280 equations in the Biosphere Model Report, and 56 compartments/158 transfers in a cut-down implementation (i.e. only representing Objects 116, 157-1 and 157-2).

Nonetheless, the AMBER implementation has largely been able to reproduce the Ecolego results almost entirely based on the description of the models and data in the supporting reports. This highlights the comprehensive way in which the models and data have been documented. The summary figures, including Figures 5-1 and 6-2 from the Biosphere Model Report, were particularly helpful.

Some notable differences arise between the AMBER and Ecolego comparisons and are discussed above.

In implementing the SR-PSU biosphere models in AMBER, a number of observations can be made about the modelling approach and associated assumptions. These are described in the sub-sections below.

2.3.1. Modelling Approach

The biosphere modelling approach adopted in SR-PSU is very complex for an assessment that covers a time-frame of tens of thousands of years. Some of the complexity cannot be justified with data; some examples are described below.

- The aquatic biosphere model distinguishes between microalgae, macroalgae and plankton, whereas data for water to primary producer concentration ratios are only available for macroalgae.
- The model for the transfer of radionuclides to agricultural soils through the use of animal manure includes a parameter that reduces the degree of contamination by a factor that reflects the fraction of radionuclides remaining in manure after fodder has passed the digestive system of cattle. The associated parameterisation is not supported by discussion of the literature; an arbitrary distribution is therefore assigned by SKB.

The biosphere model adopted by SKB for the SR-PSU assessment represents a mixture of deterministic and probabilistic approaches. The SR-PSU documentation lacks a discussion of the logic and justification for choosing probabilistic or deterministic representations of specific parameters. Some important parameters are not sampled and their uncertainty is therefore not reflected in probabilistic outputs

and associated uncertainty bands; examples include the timescales for land evolution, water flow rates and the very small well capture fractions. A very large number of other parameters are sampled.

Given the complexity of the biosphere model noted above, this means that PDFs are defined for many parameters that will have negligible importance to assessment results. A very good example is the inclusion of a PDF for the width of a barley leaf. Such detail and associated complexity is difficult to justify for calculations that extend over such long timescales, especially when other important uncertainties are not explicitly assessed.

In contrast to some of the complexity and detail in the biosphere model, other important aspects of the assessment are abstracted and simplified. The simplification of water flows provides an important example. Horizontal transport of water in sub-surface layers are neglected in the biosphere model "*for simplicity*"[2]. This has the effect of driving all advective transport to the surface regolith layer, from where horizontal advection is permitted. For C-14, this simplification is not conservative because of the very high loss rate of C-14 from the upper regolith to the atmosphere, which has a loss rate of 85 y^{-1} with best estimate parameter values. Driving C-14 towards the surface regolith layer therefore increases the loss rate to the atmosphere and reduces the amount reaching surface water. It should be noted that ingestion pathways associated with surface water dominated exposures for C-14 in previous assessments for SFR.

2.3.2. Agricultural Soil

The SR-PSU assessment adopts an abstract approach to representing radionuclide concentrations in agricultural soils. The approach uses analytical solutions to calculate radionuclide concentrations in agricultural soils. This approach enables the potential consequence of introducing agriculture to be assessed at any appropriate time after terrestrialisation, but comes at the cost of not dynamically modelling the processes involved.

In order to review the implications of the approach adopted in SR-PSU for modelling agricultural soils, an AMBER model was set up to dynamically model evolving agricultural soil concentrations. The basis for the AMBER calculation is described below.

- The evaluation is based on the modelled radionuclide release to Object 157-2 and focuses on drained mire farming.
- The dynamic model is based on that described in Section 7.2.1 of the Biosphere Model Report (illustrated in Figure 11).
- The starting concentrations and the properties of the drained mire soils were taken at 6300 AD, which is approximately the time of highest calculated doses to the drained mire farmer in the AMBER calculations described in Section 2.2.1.
- The processes illustrated in Figure 11 were explicitly modelled in AMBER; the radionuclide flux due to groundwater uptake was drawn directly from the full biosphere model for Object 157-2 described in Section 2.2.1.

[2] Section 3.2.7 of the Biosphere Model Report.

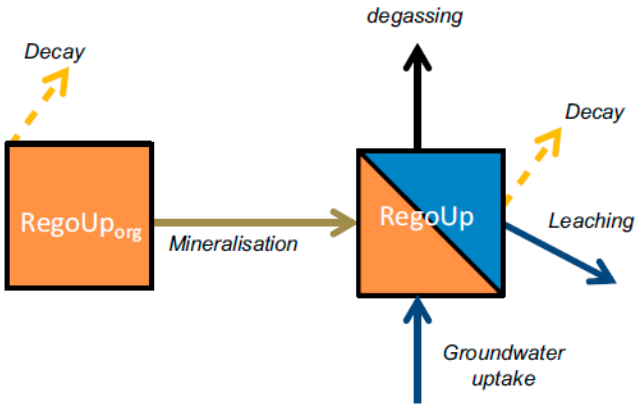

Figure 11: A graphical representation of the SR-PSU model used to simulate transport and accumulation of radionuclides in the drained mire agricultural ecosystem (Figure 7-3 from the Biosphere Model Report).

The dynamically modelled 50-year average activity concentration in the drained mire soils is compared against the result achieved with the analytical solution used in the SR-PSU modelling in Table 3.

- The comparison shows that the analytical solution provides a good approximation of the dynamically modelled results for most radionuclides (agreement within 10% for 36 out of the 43 radionuclides listed in Table 3).
- Agreement is less-good for radionuclides with half-lives less than the averaging period, with the dynamically modelled results being up to a factor of 100 greater for the shortest-lived radionuclide that is modelled (Po-210, which has a half-life of 138 days).

Table 3 also shows a comparison of the 50-year average concentration with the drained mire soil concentration at 6300 AD. This comparison shows that averaging radionuclide concentrations over 50 years only makes an appreciable difference for C-14, for which the concentrations reduce by a factor of about four. For C-14, the drained mire soil concentrations are determined by a balance between the groundwater uptake and the degassing rate, due to the very fast loss rate to the atmosphere, which has a rate coefficient in excess of 100 per year for the agricultural soils.

In calculating a 50-year average soil concentration within the SR-PSU assessment, in-growth of radioactive progeny within this timeframe is accounted for via deterministic scaling factors that are applied to the dose calculations ($doseIngrowth_{i,agri}$, Section 3.4.2 of the Biosphere Parameters Report). The effect of in-growth for each radionuclide will be dependent on retention in the soils, which, in-turn, will depend on sampled parameters including K_d. The deterministic scaling factors used in SR-PSU will therefore be inconsistent with sampled parameters used in probabilistic calculations.

Table 3: Comparison (ratios) of dynamically modelled drained mire concentrations against the analytical model used in SR-PSU. Differences greater than a factor of two are highlighted.

Radionuclide	SR-PSU Analytical Approach: 50-year Modelled Average	50-year Modelled Average: Concentration at 6300 AD
Ac227	0.49	1.02
Ag108m	1.00	0.96
Am241	1.00	0.96
Am243	1.00	1.00
C14	0.94	0.25
Ca41	0.98	0.91
Cl36	0.91	1.10
Cm245	1.00	1.00
Cm246	1.00	0.99
Cs135	1.00	1.00
Ho166m	1.00	0.98
I129	0.97	0.94
Mo93	0.99	0.99
Nb93m	0.41	1.00
Nb94	1.00	1.00
Ni59	1.00	0.99
Ni63	1.00	0.84
Np237	1.00	1.00
Pa231	0.97	1.02
Pb210	0.50	1.02
Pd107	0.99	0.99
Po210	0.01	1.02
Pu238	1.00	0.82
Pu239	1.00	1.00
Pu240	1.00	1.00
Pu241	0.38	1.00
Pu242	1.00	1.00
Ra226	0.96	1.02
Ra228	0.16	1.03
Se79	0.99	1.00
Sn126	1.00	1.00
Tc99	0.97	0.84
Th228	0.05	1.03
Th229	0.96	1.04
Th230	0.97	1.03
Th232	0.97	1.03
U232	0.96	1.04
U233	1.00	1.00
U234	0.99	1.01

Radionuclide	SR-PSU Analytical Approach: 50-year Modelled Average	50-year Modelled Average: Concentration at 6300 AD
U235	1.00	1.00
U236	1.00	1.00
U238	1.00	1.00
Zr93	1.00	0.99

Note: The results are based on the time-dependent radionuclide release from the geosphere to Object 157-2; radionuclides not applicable to that source term are therefore excluded from Table 3 (e.g. H-3 and C-60).

2.3.3. Other Specific Modelling Issues

Peat Thickness

An equation for calculating the thickness of the anoxic peat layer in the terrestrial component of the biosphere objects is presented in the Biosphere Parameters Report (Section 4.4.9). This is time dependent, as it includes the mire area in its definition. It also depends on several sampled parameters, including the density of peat ($dens_{regoPeat}$), the fraction of carbon in peat dry matter (f_{C_peat}), the fraction of refractory carbon ($f_{refrac,i}$) and the mineralisation rate of refractory carbon ($minRate_{regoPeat}$). However, the thickness of the anoxic peat layer is found to be imported as a time-dependent deterministic time sequence in the Ecolego implementation.

- In probabilistic calculations, the deterministic time-sequence for the thickness of the anoxic peat layer is inconsistent with any other parameters and processes that depend on the sampled inputs (including the transfer rates due to burial of organic matter and mineralisation, as well as activity concentrations that depend on the density of peat).
- Unlike other time-dependent inputs, the time-sequence is not presented in the Biosphere Parameters Report (Appendix C).

Litter Production in Aquatic Systems

The transfer flux due to litter production in aquatic systems includes a term (Equation 5-22, Biosphere Model Report):

$$(1 - (1 - f_{refrac,i})df_{decomp,aqu}) \quad (2)$$

where

$f_{refrac,i}$ represents the fraction of refractory carbon, and
$df_{decpmp,aqu}$ is a discrimination factor during decomposition.

For Cl-36, $f_{refrac,i}$ has a best estimate value of 0.1 for microalgae and plankton (Section 8.7.2 of the Biosphere Parameters Report), whereas $df_{decomp,aqu}$ has a best estimate value of 1.26 (Section 9.6.3 of the Biosphere Parameters Report). This combination of parameters makes the above term negative. Calculation of negative transfer fluxes indicates a fundamental conceptual problem in the representation/parameterisation of this process and should also not be permitted by the calculation tool (e.g. the AMBER software produces an error and will not solve until the flaw is rectified[3]).

[3] In the AMBER implementation, the transfer rate is set to zero for this process if the parameterisation results in a negative rate.

2.3.4. Exposure Group Assumptions

Intake fractions for the garden plot exposure group are very low. They obtain only 5% of their carbon intake from the potatoes that they grow and only 3% from the fruit and vegetables that they grow.

The fractional occupancies for the agricultural groups are also very low. The Biosphere Parameters Report (Section 10.12) states that "*historical records on work time ... were combined with estimates of the area needed to support one adult individual*". This results in an exposure time of only 54 hours per year for the drained mire farmer to grow cereals, potatoes and animal fodder. The same amount of time is assumed for the garden plot group for growing potatoes and vegetables. The number of individuals in the group is not included in the calculation of external doses (Equation 9-4 of the Biosphere Model Report), so the 54 hours per year represents an average exposure time for the whole group.

The infield, outland farmer is taken to spend 120 hours per year on arable land growing cereal and 100 hours per year harvesting hay from the wet meadows.

The agricultural exposure groups are evidently assumed to spend no other time within the contaminated regions; they are therefore assumed to live elsewhere, are not assumed to have gardens in the area and/or spend any recreational time in the area. Higher exposure times would be needed if, for example, the garden plot group were to also irrigate and fertilise areas of their garden other than that specifically used to grow the very small proportion of vegetables that they grow and consume. A survey of private wells in the local area shows that groundwater water is used to irrigate flowers etc. (Ludvigson, 2002).

The hunter-gatherer group obtains only a very small proportion of their dietary intake from Object 157-2, which receives the contaminated discharges from the geosphere. After terrestrialisation, only 0.7% of the hunter-gatherer group's dietary intake comes from Object 157-2 with best estimate assumptions. This percentage is inversely proportional to the number of individuals in the exposure group (see Equation 9-12 of the Biosphere Model Report). Including the equivalent of 30 adult individuals in the definition of the hunter-gatherer group therefore dilutes exposures in comparison to other groups.

2.3.5. Editorial Observations

Editorial omissions and comments relating the SR-PSU reports are described below.

Half-lives and dose coefficients:

- Table 3-1 of the Biosphere Parameters Report, which lists the safety relevant radionuclides, is missing Th-232 and Ra-228. Both are identified as being explicitly modelled in the 4N chain in Table 3-1 of the Radionuclide Transport Report.
- Table 3-3 of the Biosphere Parameters Report and Table 3-4 of the Data Report (SKB, 2014d) are missing half-life data for Th-232 and Ra-228.
- Half-lives for Ac-227, Cm-242, Pa-231, Pb-210, Po-210, Ra-226, Th-228, Th-229, Th 230, U-233 are not available in Table 3-4 of the Data Report, though values are available in the Biosphere Parameters Report.
- The half-lives "recommended for use in SR-PSU" in Table 3-4 of the Data Report differ in many cases from those listed against the dose coefficients

in Tables 3-3 and 3-4 of the Biosphere Parameters report (the AMBER model uses the Data Report in preference).
- Dose coefficients for Th-232 and Ra-228 are missing in Tables 3-5 and 3-6 of the Biosphere Parameters Report and are instead obtained from source literature in the AMBER implementation.

Regolith properties:
- The discussion of peat density in Section 5.3.4 of the Biosphere Parameters report notes that "*both density and porosity of peat is believed to be related to the successional stage of the mire and consequently the peat in a mire may follow a gradient from minimum to maximum*". This indicates that time-dependent density and porosity would be appropriate for peat. However, the above text is used by SKB to justify sampling from a uniform distribution without time-dependency, the logic of which is difficult to follow.
- The soil diffusivity of CO_2 is shown to vary from 0.5 $m^2\ y^{-1}$ to 69.5 $m^2\ y^{-1}$ in Table 5-12 of the Biosphere Parameters Report, a range of about two orders of magnitude. However, the geometric standard deviations (GSDs) assigned to the log-normal distributions range from 3.2 to 4.5. These GSDs are inconsistent with the minimum and maximum values that are reported, because they imply statistical distributions covering many orders of magnitude. It is possible that the GSD has been misinterpreted in this case, which suggests that it could be equally misinterpreted for other parameters.

Aquatic parameters:
- Some of the parameter names described in the text have become inconsistent with the parameter names described in the associated tables. For example, the mineralisation rates of organic carbon in particulate matter in the water column in lakes and marine basins are assigned names of minRate_water_PM_lake and minRate_water_PM_sea in the text of Section 8.7.3 of the Biosphere Parameters Report, but shown as minRate_PM_lake/sea in the associated Table 8-4.

Terrestrial parameters:
- The units in Table 9-18 of the Biosphere Parameters Report, which describes the mineralisation rate for peat (kgC kgC and kgC kgC y^{-1}), are inconsistent with the title for the table (kgC kgC^{-1} y^{-1}) and inconsistent with the associated text.
- The model includes a sampled parameter that defines the fraction of radionuclides remaining in manure after fodder has passed through the digestive system of cattle. This has a reference value of 1 and is assigned a uniform range from 0.8 to 1 without discussion. This parameter is illustrative of over-complexity in the biosphere modelling for SR-PSU. In typical biosphere assessments, any losses between ingestion by animals and use of their waste as fertiliser are reasonably and slightly conservatively ignored.

Exposure equations:
- The calculation of radionuclide concentrations in milk requires the concentration of carbon in milk expressed in terms of kgC L^{-1} (Equation 9-36 of the Biosphere Model Report). However, the Biosphere Parameters Report gives the units for the parameter conc_C_milk as

kgC $kgfw^{-1}$. The density of milk is therefore needed and is omitted from Equation 9-36.

- The Biosphere Parameters Report does not include data for the fraction of the fuel inventory that ends up in ash and gas after combustion of wood or peat (*f_combust*). The AMBER implementation uses value distributions obtained directly from the Ecolego model, which specifies uniform distributions: 0.5 [0.25 to 0.75] for all elements except carbon, and 0.95 [0.9 to 0.99] for carbon.

3. Biosphere Model for C-14

In the SAR-08 assessment (Bergström et al., 2008), ingestion of C-14 in contaminated fish was one of the key exposure pathways. In the SR-PSU assessment, only the hunter-gatherer group includes ingestion of fish and crayfish. Table 4 summarises the contribution of C-14 to the most exposed group in each of the SR-PSU calculation cases.

Table 4: Summary of contributions of C-14 to peak dose for the SR-PSU calculation cases

Calculation case	C-14 contribution (%)	Biosphere object	Most exposed group
CCM_GW	17.9 (C-14 org)	157_2	Drained mire farmer
CCM_TR	17.9 (C-14 org)	157_2	Drained mire farmer
CCM_EP	88.8 (C-14 org) 10.7 (C-14 inorg)	114	Hunters and gatherers
CCL_IH	8.4 (C-14 org)	157_2	Drained mire farmer
CCL_FH	17.4 (C-14 org)	157_2	Drained mire farmer
CCL_BC	17.0 (C-14 org)	157_2	Drained mire farmer
CCL_BB	17.9 (C-14 org)	157_2	Drained mire farmer
CCL_EQ	9.0 (C-14 org)	157_2	Drained mire farmer
CCL_CA	< 1	157_2	Drained mire farmer
CCL_WD	13.7 (C-14 org)	-	Garden plot
CCL_WI	5 to 59.9% (C-14 org) for SFR 1 [4]	-	Garden plot
CCC_S1	10.3 (C-14 org) 3.9 (C-14 inorg)	157_2	Drained mire farmer
CCC_S2	< 1	157_2	Drained mire farmer

In this Section consideration is given separately to the general representation of C-14 in the aquatic (Section 3.1) and terrestrial (Section 3.2) ecosystems in the SR-PSU assessment. This includes a review of the representation of biosphere features, events and processes (FEPs) in both ecosystems. Specific consideration is then given to the atmospheric sub-model (Section 3.3), and the modelling of interactions between the atmosphere and both the aquatic and terrestrial ecosystems.

3.1. The Aquatic Ecosystem

In this section, an overview of the model for the aquatic ecosystem is given (Section 3.1.1), along with an audit of the representation of FEPs in this ecosystem. The parameterisation of aquatic litter respiration and accumulation in sediments is discussed in Section 3.1.2. These are considered here as neither process was included in the model for C-14 in aquatic ecosystems in the SAR-08 assessment. Given the dominance of ingestion of C-14 contaminated fish on the human dose in the SAR-08 assessment (Bergström et al., 2008), the modelling of the uptake of C-14 into biota and humans in the aquatic ecosystem is discussed in Section 3.1.3.

[4] The value is dependent on waste vault intruded (Silo, 1BMA, 1BLA, 1BTF or 2BTF). Calculated doses from C-14 from the other waste vaults make a non-significant contribution to the total calculated doses associated with releases from those vaults.

3.1.1. Overview

A summary of the FEPs described in Biosphere Model Report for the aquatic ecosystem is given in Table 5. The FEP IDs are based on their mapping in Table 2-1 in the Biosphere FEP Handling Report, and the summary of the processes in Table 3-1 of the Biosphere Model Report.

The following inaccuracies are highlighted in the review of the FEP handling logic.

- Burial: Has been mapped to "Deposition", but that relates to transfer of material to a surface, not below that surface.
- Mineralisation: Has been mapped to "Decomposition". However, the term is not linked with any of the FEPs in either the Biosphere FEP Report or Biosphere FEP Handling Report.

Furthermore, it is not always clear where each of the processes sit in the interaction matrix of Appendix B of the Biosphere Model Report, i.e. exactly which compartments are affected by that process. Thus, despite the use of FEPs in the biosphere being described in two separate reports, there is not a transparent alignment between processes described in the Biosphere Model Report and the FEPs identified in the Biosphere FEP Report and Biosphere FEP Handling Report.

Table 5: Summary of FEPs in the Aquatic Ecosystem relevant to C-14

FEP	FEP ID [5]	Transfer from	Transfer to
Advection	Bio32	Several [6]	
Diffusion	Bio32	Several [6]	
Plant uptake	Bio22	Surface water	Primary producers
Litter respiration	Bio02, Bio03, Bio04	Primary producers	Surface water
Litter production	Bio03, Bio05, Bio12	Primary producers	Sediment (RegoUp_org)
Sedimentation	Bio34	PM PM_org	RegoUp RegoUP_org
Resuspension	Bio39	RegoUp RegoUP_org	PM PM_org
Burial	Bio34	RegoUp RegoUP_org	RegoPG RegoPG_org
Bioturbation	Bio01	RegoPG RegoPG_org	RegoUp RegoUP_org
Mineralisation	Bio04	PM_org RegoUp_org RegoPG_org	Surface water RegoUp RegoPG
Degassing	Bio24	Surface water (gas dissolved in)	Atmosphere
Gas uptake	Bio24	Atmosphere	Surface water (gas dissolved in)

The SR-PSU assessment differs from previous SKB assessments in as much as losses to the atmosphere above the water body are considered in the conceptual model, with a two-way exchange process invoked. In addition, the process of litter

[5] The FEP ID is as given in the Biosphere FEP Handling Report.

[6] The following two-way transfers are included: Water ↔ RegoUp, RegoUp ↔RegoPG, RegoPG ↔ RegoGL, and RegoGL ↔ RegoLow.

production as a result of the degradation of primary producers, and an exchange with particulate matter in the water body, provides a means of C-14 being recycled in the upper sediments via the upper regolith compartments (Figure 12). Thus, whereas previous SKB assessments have had a "single pass" model for C-14 in water bodies, the SR-PSU model has two means of recycling the C-14 in the water.

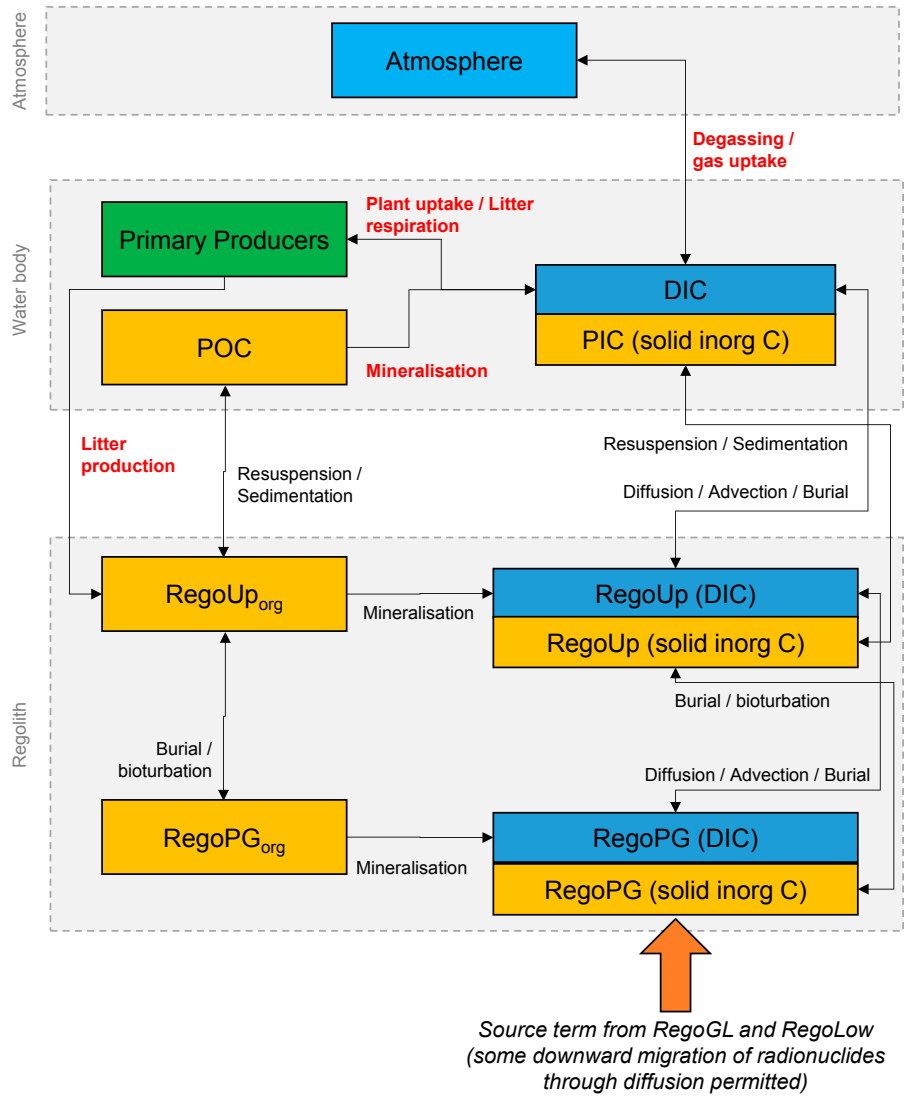

Figure 12: Schematic representation of the radionuclide model for the aquatic biosphere, including source term[7] (based on Figure 2-2 of the K_d and CR Report). Transfers highlighted in red have a specific parameterisation for C-14.

[7] "Rego" refers to regolith layers; PG refers to post-glacial deposits; GL refers to glacial clay; the subscript "org" refers to organic matter; Up refers to the upper sediment layer; PIC refers to particulate organic matter; and DIC refers to dissolved inorganic carbon.

3.1.2. Aquatic Litter Respiration and Accumulation in Sediments

On an annual timescale, the SR-PSU assessment assumes that the primary producer biomass is in equilibrium, i.e. that net primary production is balanced with an equal loss of biomass through consumption and litter production (Section 5.2.2 of the Biosphere Model Report). Litter respiration is considered as being equivalent to the fraction of litter production of non-refractory organic plant material (i.e. the refractory fraction is resistant to degradation). In aquatic ecosystems, the smaller the percentage refractory organic matter in litter (*f_refrac*), the greater the release to the water.

Distributions of refractory organic matter are defined for each of the three primary producer types (macroplankton, microplankton and phytoplankton), although the same distributions are assumed across both marine and freshwater ecosystems (Table 6).

Table 6: Distribution of f_refract in aquatic ecosystems assumed in SR-PSU.

Ecosystem	Distribution	Mean	Minimum	Maximum
Microplankton	Uniform	0.1	0.01	0.25
Macroplankton	Uniform	0.3	0.2	0.4
Phytoplankton	Uniform	0.1	0.01	0.25

Thus, although some of the C-14 associated with the primary producers is assumed to accumulate in sediment, the overall percentage is 30% or lower in the deterministic calculations. The C-14 released back to the water body would be able to leave the system more rapidly via advective transport to an adjacent biosphere object, and potentially through degassing to the atmosphere.

3.1.3. Uptake into Aquatic Biota and Humans

Whereas, in the SR-Site assessment, the calculation of radionuclide concentrations in aquatic primary producers amalgamated the three groups (benthic microplankton, benthic macroplankton, and phytoplankton) together, they have been modelled separately in the SR-PSU assessment. The specific activities of C-14 in fish and crayfish in the SR-PSU assessment are equated to a weighted average of the specific activity of the three primary producers.

Using the concentration of C-14 in water in biosphere object 157_1 (Bq m^{-3}) calculated in Ecolego and the calculated concentration in fish in that object (Bq kgC^{-1}) it is possible to derive a water-to-fish concentration ratio (CR) for comparison with those given in IAEA (2010) and IAEA (2004), for limnic and marine ecosystems respectively, allowing for conversion between kgC and kg fresh weight (fw). Appendix F of the K_d and CR report provides dry matter (0.25 kg dw kg^{-1} fw) and carbon content (0.47 kgC kg^{-1} dw) conversion factors for fish, both of which derive from IAEA (2010).

Table 57 of IAEA (2010) recommends a mean CR value of 400 m^3 kg^{-1} fw for carbon in fish muscle in limnic ecosystems. Table III of IAEA (2004) recommends a CR of 20 m^3 kg^{-1} fw for carbon in fish muscle in marine ecosystems. By contrast, the effective CRs calculated in Ecolego for biosphere object 157_1 are 10.7 m^3 kg^{-1} fw during the evolution of the marine phase of the biosphere object, dropping to 5.3 m^3 kg^{-1} fw once the bay becomes isolated (Figure 13). The values modelled in

SR-PSU are therefore significantly lower than if a concentration ratio approach was adopted based on IAEA recommendations.

Two of the parameters considered by SKB to most affect the uncertainty in the calculated dose associated with fish consumption (see Appendix F (p299) of the Radionuclide Transport Report) are the fraction of H_2CO_3 in the soil and also the lake (f_H2CO3_ter and f_H2CO3_lake). These two parameters are discussed in more detail in Section 3.3.2.

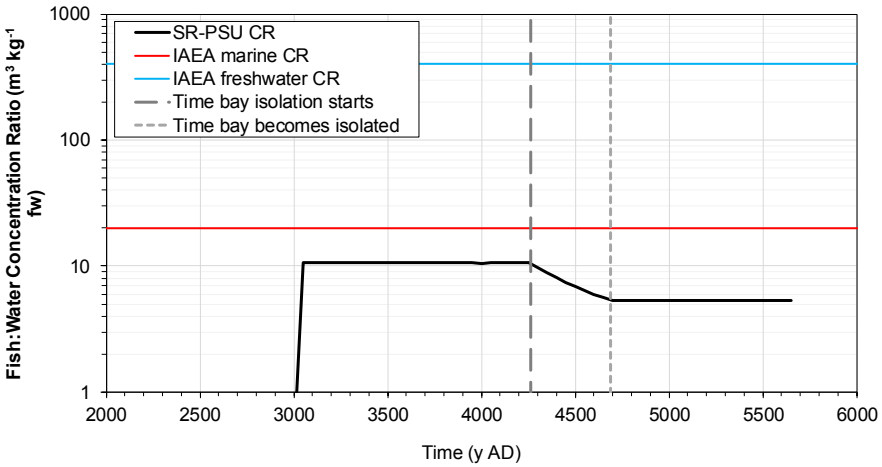

Figure 13: Fish:water concentration ratio (CR, m^3 kg^{-1} fw) modelled for Object 157_1 in SR-PSU compared against IAEA recommended values. Note the logarithmic y-axis.

Using the same methodology for the aquatic primary producers yields calculated CRs in biosphere object 157_1 of 7.0 m^3 kg^{-1} fw during the evolution of the marine phase of the biosphere object, dropping to 3.5 m^3 kg^{-1} fw once the bay becomes isolated. IAEA (2004) recommends values of 20, 10 and 9 m^3 kg^{-1} fw for macroalgae, zooplankton and phytoplankton in a marine ecosystem, respectively. IAEA (2010) recommends a mean value of 16 m^3 kg^{-1} for edible freshwater aquatic plants. The values modelled in SR-PSU are therefore again lower than those that would be adopted based on IAEA recommended concentration ratios.

3.2. The Terrestrial Ecosystem

In this section, an overview of the model for the terrestrial ecosystem is given in Section 3.2.1, along with an audit of the representation of FEPs in this ecosystem. Specific consideration is then given to the modelling of the accumulation and degradation of organic matter in Section 3.2.2. Terrestrial litter respiration is discussed in Section 3.2.3. Neither process was given explicit, or implicit, consideration in the SAR-08 assessment.

3.2.1. Overview

One of the key differences between the SR-PSU model for terrestrial C-14 and that used in previous SKB assessments is the explicit inclusion of organic carbon pools in the dynamic compartment models. This relates only to organic matter presumed to be present in the regolith already, or that arising from the decomposition of

primary producers. All three forms of carbon in the waste inventory (C-14 org, C-14 inorg, and C-14 ind)[8] are assumed to enter the biosphere as dissolved inorganic carbon (DIC), and are all treated identically within the biosphere model itself.

The terrestrial ecosystem modelling is described in two separate chapters in the Biosphere Model Report, one covering mire ecosystems and one covering agricultural ecosystems. The latter is split further to cover three types of agriculture separately: infield-outfield agriculture, drainage and cultivation of a lake-mire system and garden plot cultivation.

A summary of the FEPs relating to C-14 described in Biosphere Model Report for the four terrestrial ecosystem types is given in Table 7, Table 8, Table 9 and Table 10. The FEP IDs are based on their mapping in Table 2-1 and Table 3-3 in the Biosphere FEP Handling Report, and the summary of the processes in Table 3-1 of the Biosphere Model Report.

The following issues are highlighted in the review of the FEP treatment.

- Table 3-1 of the Biosphere Model Report explicitly states that litter respiration/release is not considered in the radionuclide flux calculations for agricultural ecosystems, yet Section 7.1.3 of the same report describes the litter respiration/release process in the infield-outland agriculture system.
- Fertilisation and releases to the atmosphere from combustion can be considered as anthropogenic releases and, as such, are processes that link humans with environmental media (see Table 8 and Table 10). However, the material and radionuclide transport does not reflect a transfer from a human pool/compartment, but represents transfers from other biosphere media (notably primary producers).
- Although "Terrestrialisation / ingrowth of mire vegetation" (Table 7) is mapped to Primary Production (Bio13) and Covering (Bio33) in the Biosphere Model Report, it is not clear as to which processes it affects in the interaction matrix.
- It is not clear to which FEP "Leaf degassing" maps. Presumably it is phase transition (Bio24), but that is not included for the 6:5 (primary producer: local atmosphere) cell of the interaction matrix in Appendix B of the Biosphere Model Report. Furthermore, leaf degassing is not given explicit mention in either the Biosphere FEP Report or the Biosphere FEP Handling Report.
- It is not entirely clear as to how "Groundwater uptake" in drained mires used for agriculture (Table 9) maps to any of the processes listed in either the Biosphere FEP Report or the Biosphere FEP Handling Report, though this may be Import (Bio36) based on Table 3-1 of the Biosphere Model Report.
- Plant uptake of C-14 in the canopy atmosphere is described with a stable carbon flux in atmosphere model description (Section 8.1.3 of Biosphere Model Report), yet is described as a transfer process only for the mire ecosystem (Section 6.2.1 of the Biosphere Model Report). It is only by looking at the Ecolego model that it becomes clear that atmospheric uptake of C-14 is considered in all four terrestrial ecosystems. Such omissions in the documentation cannot be readily explained when other processes, such as mineralisation and degassing, are explicitly described for all four terrestrial ecosystems.

[8] Organic C-14, inorganic C-14, and radiologically induced C-14.

- Finally, the two-way interaction between soil and atmosphere applies only to the mire ecosystem.

Table 7: Summary of FEPs in the Terrestrial Ecosystem relevant to C-14 - Mire

FEP	FEP ID	Transfer from	Transfer to
Advection	Bio32	Several [9]	
Diffusion	Bio32	Several [9]	
Plant uptake	Bio13, Bio15	Atmosphere RegoUp (dissolved)	Primary producers Primary producers
Litter respiration	Bio02, Bio03, Bio04	Primary producers	Atmosphere
Litter production	Bio03, Bio05, Bio12	Primary producers	RegoUp_org
Burial	Bio34	RegoUp RegoUP_org	RegoPG RegoPG_org
Mineralisation	Bio04	RegoUp_org RegoPG_org	RegoUp RegoPG
Degassing	Bio24, Bio32	RegoUp (gas dissolved in pore water)	Atmosphere
Gas uptake	Bio24	Atmosphere	Surface water (gas dissolved in)
Terrestrialisation/ ingrowth of mire vegetation	Bio13, Bio33	RegoUp_aqu, RegoPG_aqu RegoUp_org_aqu, RegoPG_org_aqu	RegoPG RegoPG_org

Table 8: Summary of FEPs in the Terrestrial Ecosystem relevant to C-14 – Infield-outfield agriculture

FEP	FEP ID	Transfer from	Transfer to
Advection	Bio32	As Table 7	As Table 7
Diffusion	Bio32	As Table 7	As Table 7
Fertilisation	Bio16, Bio38	Humans	RegoUp, RegoUp (water)
Litter respiration	Bio02, Bio03, Bio04	Primary producers	Atmosphere
Litter production	Bio03, Bio05, Bio12	Primary producers	RegoUp_org
Leaching	Bio24	RegoUp (water)	RegoPG (water)
Mineralisation	Bio04	RegoUp_org	RegoUp
Degassing	Bio24, Bio32	RegoUp (gas dissolved in pore water)	Atmosphere

[9] The following two-way transfers are included: RegoUp ↔ RegoPG, RegoPG ↔ RegoGL, and RegoGL ↔ RegoLow.

Table 9: Summary of FEPs in the Terrestrial Ecosystem relevant to C-14 – Drainage and cultivation of a mire

FEP	FEP ID	Transfer from	Transfer to
Advection	Bio32	As Table 7	As Table 7
Diffusion	Bio32	As Table 7	As Table 7
Groundwater uptake	?	RegoUp	RegoUp
Leaching	Bio24	RegoUp (water)	RegoPG (water)
Mineralisation	Bio04	RegoUp_org RegoPG_org	RegoUp RegoPG
Degassing	Bio24, Bio32	RegoUp (gas dissolved in pore water)	Atmosphere

Table 10: Summary of FEPs in the Terrestrial Ecosystem relevant to C-14 – Garden plot cultivation

FEP	FEP ID	Transfer from	Transfer to
Advection	Bio32	As Table 7	As Table 7
Diffusion	Bio32	As Table 7	As Table 7
Fertilisation	Bio16, Bio38	Humans	RegoUp, RegoUp (water)
Irrigation	Bio16	*Irrigation water*	RegoUp
Leaf retention	Bio37	RegoUp (water)	Primary producers
Leaf degassing	?	Primary producers	Atmosphere
Leaching	Bio24	RegoUp (water)	RegoPG (water)
Mineralisation	Bio04	RegoUp_org RegoPG_org	RegoUp RegoPG
Degassing	Bio24, Bio32	RegoUp (gas dissolved in pore water)	Atmosphere
Release to atmosphere from combustion	Ter15, Ter25	Humans	Atmosphere

3.2.2. Accumulation and Degradation of Organic Matter

The processes involving accumulation and degradation of organic matter are central to the behaviour of C-14. The accumulation of soil organic matter, and C-14 associated with this organic matter, results from the addition to the soil surface of plant litter containing carbon 'fixed' from atmospheric CO_2 in the vegetation canopy plus decay of below-ground root biomass, which is also ultimately derived from atmospheric CO_2. This 'fixed' carbon is otherwise referred to as 'Net Primary Productivity' (NPP) and represents the primary input of organic matter into the ecosystem. In wetland ecosystems, it is the flow of organic matter from canopy to ground surface that results in the accumulation of large stocks of organic matter in the form of peat, since the decomposition rate of the deposited organic matter in wet (and cold) conditions is very slow compared with relatively dry (and/or warm) ecosystems.

The SR-PSU assessment assumes that C-14 in groundwater and soil pore water is in the form of dissolved inorganic carbon (H_2CO_3, HCO_3^-, CO_3^{2-} and CO_2), the

proportions of which are both pH- and temperature-dependent (max, median and min values are calculated for old, 'middle-aged' and young wetlands, respectively, since pH is assumed to decrease as the age of a mire increases). The transport of low molecular weight organic carbon species (methane, acetate and formate, all in dissolved form) is mentioned in the Biosphere Model Report but these are considered to be mineralised so quickly that they are rapidly converted into inorganic carbon species:

"*Dissolved low molecular weight organic carbon is typically mineralised within days or weeks (Howard 1991), and all C-14 released to the aqueous phase is therefore assumed to be transformed to inorganic carbon within the yearly time resolution of the model.*" (Biosphere Model Report, 5.1.1, p. 46).

Direct transport of gaseous carbon species (CO_2 and CH_4) from the subsurface does not appear to be considered. Furthermore, any description or consideration of the role of $^{14}CH_4$ as a dose-forming species of C-14 is completely absent. $^{14}CH_4$ may not form in the repository itself, but it will be produced in anoxic sub-soil or in anaerobic microsites within soil crumbs. Methane can be formed by either the hydrogenotrophic or acetogenic pathways, which convert CO_2 or acetic acid (CH_3COOH), respectively, to CH_4 as a result of the action of anaerobic bacteria (methanogens – see Figure 14). It is acknowledged in the Biosphere Model Report (Section 5.1.1) that dissolved methane and acetate (which is a precursor of methane formation via the acetogenic pathway) can be transported from the deep groundwater, which gives rise to the potential for either the direct transport of $^{14}CH_4$ into the biosphere from the geosphere or the formation of $^{14}CH_4$ in anoxic sites within the biosphere following transport of C-14 labelled acetate originating from the geosphere. Furthermore, SKB have themselves noted the presence of large amounts of methane in sediments of lakes and shallow bays in the Forsmark area (Borgiel, 2004; Karlsson and Nilsson, 2007).

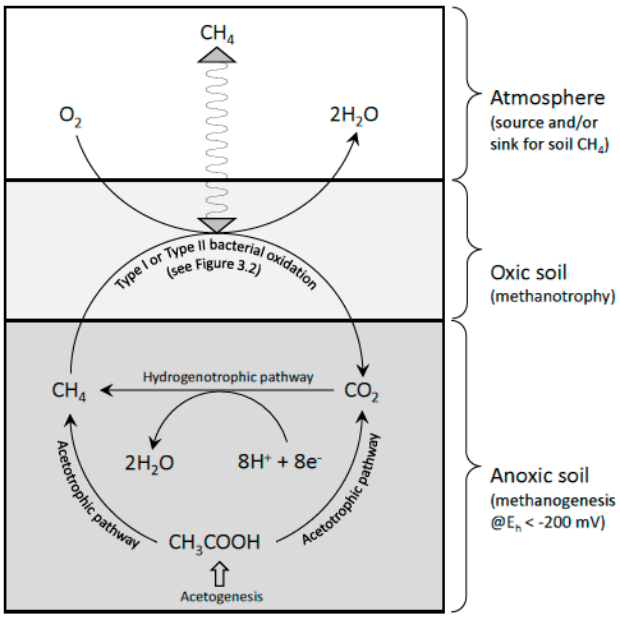

Figure 14: Pathways of methane production (methanogenesis) and oxidation (methanotrophy) in anoxic and oxic soils, respectively (from Shaw and Thorne, 2016).

This potential formation of $^{14}CH_4$ appears to have been missed in the SR-PSU assessment, or to have been judged to be insignificant[10]. If it has been judged to be insignificant, this needs to be stated clearly in the description of the radionuclide transport model and the processes it represents, in the Biosphere Model Report.

In the agricultural ecosystem, a steady state activity concentration of C-14 will be reached as the inputs in the form of fertiliser (animal manure) are balanced by losses from 'radioactive decay, leaching and degassing'. Losses of C-14 in the form of microbiologically-respired CO_2 are considered to be so fast ("*within the order of a year*") that 'litter respiration' (Litter_resp = Bq/y) is not represented by a rate coefficient. Instead, it is calculated on the basis of what remains after taking into account the fraction of 'recalcitrant' organic matter that enters the soil (e.g. Equation 7-8 in the Biosphere Model Report, p. 73).

According to Jenkinson and Rayner (1977), soil organic matter can be broken down into the following five discrete fractions, each with its own characteristic degradation half-time (Table 11):

- decomposable plant material (DPM);
- resistant plant material (RPM);
- soil biomass (BIO);
- physically stabilised organic matter (POM); and
- chemically stabilised organic matter (COM).

According to the rate coefficient for DPM proposed by Jenkinson and Rayner, freshly added plant litter would indeed be almost completely degraded in around one year (T0.99 = 1.1 year). However, it is not entirely clear from the model description in Figure 7-2 of the Biosphere Model Report whether 'hay fertilisation' refers to the addition of fresh hay or animal manure (which is essentially 'processed' hay). If it referred to animal manure, then much of the readily decomposable carbon (including C-14) will already have been removed in the animals' gut and the characteristics of the 'hay' added to the soil will be more similar to the RPM in Table 11 (T0.99 = 15.35 year). This would lead to an underestimation of the build-up of C-14 in soil organic matter. This could be addressed by assigning an explicit rate coefficient for the decomposition of organic matter in the form of hay/manure.

Table 11: Original data from Jenkinson and Rayner (1977) are presented in the shaded column; rate coefficients (k), T0.9 and T0.99 values (times to degrade organic matter by 90% and 99%, respectively) have been calculated from the T½ values.

Fraction	k (y^{-1})	T ½ (y)	T 0.9 (y)	T 0.99 (y)
DPM	4.20	0.17	0.55	1.10
RPM	0.30	2.31	7.67	15.35
BIO	0.41	1.69	5.61	11.23
POM	0.014	49.5	164.4	328.9
COM	0.0004	1980	6577	13155

Any organic carbon that is not rapidly decomposed is considered to be 'refractory'. Refractory organic carbon is defined in the Biosphere Parameter Report (8.7.2) as

[10] This seems to have occurred, despite the Biosphere FEP Report noting that the excretion of methane, and carbon dioxide, from decomposers should be considered explicitly in the SR-PSU assessment its discussion of transfers between 7:5 (decomposers affecting gas and local atmosphere).

"*the part of the primary production NPP that is not decomposed or exported, but contributes to the sediment accumulation of organic carbon, i.e. the refractory organic matter left after initial mineralisation*."

Refractory organic matter does decompose, but much more slowly than the non-refractory organic matter fraction. The decomposition of refractory organic matter is assigned a rate called MinRate: values for this parameter are given in Table 9-18 of the Biosphere Parameter Report (p. 110) and are shown here in Table 12.

Table 12: Rate coefficients for the decomposition of refractory organic matter (from Table 9-18 of Biosphere Parameter Report) are presented in the shaded column; T½, T0.9 and T0.99 values (times to degrade OM by 50%, 90% and 99%, respectively) have been calculated from the rate coefficients.

Fraction	k (y^{-1})	T ½ (y)	T 0.9 (y)	T 0.99 (y)
Drained Mire	0.007	99.02	328.9	657.9
Garden Plot	0.0029	239.0	794.0	1588
Infield Outland	0.0029	239.0	794.0	1588
Mire (RegoUP)	0.0029	239.0	794.0	1588
Mire (RegoPG)	0.00007	10664	35424	70849

According to the data in Table 12, the decomposition half-times for recalcitrant organic matter in the SR-PSU assessment range from 99 to 10,664 years. This compares with Jenkinson and Rayner's estimated degradation half-times for physically-stabilised (POM) and chemically-stabilised (COM) organic matter of 50 to 1980 years, as shown in Table 11. The largest SR-PSU half-time estimate (10,664 years) is for decomposition of recalcitrant OM under anoxic conditions in mires, whereas Jenkinson and Rayner's estimates were for oxic agricultural soils in which aerobic decomposition would be expected to be faster. Excluding this upper value, the range in Table 12 is from approximately 99 to 240 years, which lies between Jenkinson and Rayner's degradation half-times for POM and COM. The mineralisation rates used in SR-PSU are therefore considered to be reasonable.

3.2.3. Terrestrial Litter Respiration

As noted in Section 6.2.2 of Biosphere Model Report, on an annual timescale it is assumed that the primary producer biomass is in equilibrium, i.e. that net primary production is balanced with an equal loss of biomass through consumption and litter production. Litter respiration is considered as being equivalent to the fraction of litter production of non-refractory organic plant material; the refractory organic matter is assumed to enter the soil. Therefore, as in the aquatic system, the smaller the percentage refractory organic matter (*f_refrac*), the greater the release to the inorganic upper regolith compartment.

In the Biosphere Model Report, terrestrial litter respiration is assumed to occur in both the mire and in the infield-outland agriculture systems only.

In the terrestrial ecosystem, the best estimate value of the fraction of refractory organic matter is assumed to be 30%, with a uniform distribution of 5% to 50%, based on the mass of litter remaining in a number of different peatland decay experiments over a 10 year period. Examination of the values used in Ecolego

indicates that in the 1000 realisations the range of *f_refrac* used for terrestrial systems was 13.8 to 35%[11], with an arithmetic mean of 27.1%.

The range that SKB have defined for the fraction of refractory carbon in the mire soils does not cover the slow decay of *Sphagnum* moss, which one would expect to observe in wetlands. For example, based on the exponential decay rates of 0.03 to 0.08 y^{-1} cited in Moore and Basiliko (2006), one would expect 45 – 74% refractory organic matter to be remaining after 10 years of decay. Furthermore, the refractory organic matter content of peatland vegetation may not be appropriate for agricultural crops or forests.

Harmon et al. (2009) considers the decay of a range of plant types over a 10 year period, including various trees species (*Quercus*, *Pinus spp.*, *Acer*), grasses and wheat, at a variety of latitudes and climatic zones in North and Central America. Disregarding the tropical *Drypetes glauca*, the geometric mean of the mass left after 10 years is 23.6%, with a range of 0.03 – 79.7%. Qualls (2016) has monitored the decomposition rates of forest floor organic matter in both coniferous and deciduous watersheds in North Carolina over a 13 year period. After 10 years the mass of carbon remaining was typically around 20% or less.

3.3. The Atmospheric Sub-Model

As part of the SR-PSU assessment, the radionuclide transport model has been enhanced over that used in the SR-Site assessment to better represent the transport and accumulation of C-14 in the surface systems[12].

At the time of the Initial Phase Review, only a summary of the new atmospheric sub-model was provided in the Biosphere Model Report[13]. It described how the new model had been developed specifically to address $^{14}CO_2$ exchange and uptake between soil-vegetation-atmosphere in the terrestrial ecosystem and water-atmosphere in the aquatic ecosystems. In Section 8.9 of Biosphere Model Report, it is stated that, with respect to the atmospheric model "*a more complete description of the relatively simple models, and a comparison with more detailed, process-oriented models, can be found in Avila and Kovalets (2014)*". However, the Avila and Kovalets report was not published until November 2016, and more details are given as to the assessment model in Section 8 of Biosphere Model Report than Section 2 of Avila and Kovalets (2016). Specifically, it is only in the Biosphere Model Report where release rates to the atmosphere are defined.

Section 3.3.1 provides an overview of the new atmospheric model. In Section 3.3.2 the conceptual model of the degassing of C-14 from the surface, and its parameterisation in the mathematical model, are discussed.

3.3.1. Overview

The atmospheric model for C-14 developed for SR-PSU (Avila and Kovalets, 2016) is very different to that used in the SAR-08 or SR-Site assessments, the latter being

[11] This parameter seems to be in the "parameters rejected" selection in the Ecolego file, but there is no explanation as to what has happened to those parameters, or why they were rejected.
[12] Section 1.5 of the Main Report.
[13] Section 8 of the Biosphere Model Report.

documented in Avila and Pröhl (2008). The new atmospheric exchange model reflects an acknowledgement of micrometeorological processes. Similar models have been adopted by other waste management organisations in support of their safety assessments over recent years.

As was noted in the Initial Phase Review (SSM, 2016), with regards to terrestrial ecosystems, whereas a single compartment was used for the above-ground atmosphere in the model developed by Avila and Pröhl (2008), in the SR-PSU assessment this has been split into three compartments, with the total height (10 m) being equivalent to that of agricultural land in Avila and Pröhl (2008). With regards to aquatic ecosystems, in Avila and Pröhl (2008) the atmosphere above the water body was disregarded, whereas in SR-PSU there are two compartments, with a total height of 10 m, equivalent to that the of terrestrial atmosphere.

C-14 is assumed to enter the terrestrial atmosphere via degassing from the soil. In aquatic ecosystems, C-14 is assumed to enter the atmosphere as a consequence of degassing from the water body surface. The process of degassing is discussed in more detail in Section 3.3.2 below.

The turbulent mixing between atmospheric layers is based on the well-established resistance analogue model developed by Shuttleworth and Wallace (Shuttleworth and Wallace, 1985; Shuttleworth and Gurney, 1990). No further consideration is therefore given to the modelling of turbulent mixing of the atmospheric compartments in this review.

With respect to advective losses of C-14 from each atmospheric layer, the same basic principles used in Avila and Pröhl (2008) are used in the SR-PSU assessment, but with a more involved definition of the wind speed. Specifically, it is assumed that wind speed increases in a logarithmic manner above the height of the displacement plane. Again, this is something which has been considered previously by other waste management organisations.

Although the model described in the Biosphere Model Report describes a two-way gas exchange between the surface and the lower atmosphere compartment, the uptake of gas by the upper regolith or water is disregarded in the calculation of the specific activity of C-14 in the lower atmosphere.

3.3.2. Degassing of soils and surface water bodies

Degassing of C-14 from mire and agricultural soils is presented in Sections 6.2.6 and 7.1.7 of Biosphere Model Report, respectively. Degassing from water bodies is discussed in Section 5.2.10 of Biosphere Model Report.

SKB have used the same model for degassing from water bodies and mire soils. In particular, the flux of C-14 into the atmosphere as a result of degassing from these is proportional to the fraction of dissolved inorganic carbon that is in the form of CO_2/H_2CO_3 (f_{H2CO3}), and the gas exchange coefficient (also described as the piston velocity).

Fraction of dissolved inorganic carbon that is in the form of CO_2/H_2CO_3 (mires and water bodies)

f_{H2CO3} is defined according to an expression that depends on the temperature dependent dissociation constants of HCO_3^- and CO_3^{2-} and the concentration of H^+.

The dissociation constants used in both marine and limnic ecosystems were based on values derived at 25ºC (Weiss, 1974; Prieto and Millero, 2002). The source of the dissociation constants used in calculating f_{H2CO3} for the terrestrial ecosystem is not clear, although a temperature of 15ºC was used. The distributions of f_{H2CO3} for the three basic ecosystem types by SKB for the SR-PSU assessment are given in Table 13, which are based on the pH and temperature variations in the ice-free season.

Table 13: Distribution of f_{H2CO3} assumed in the SR-PSU assessment

Ecosystem	Distribution	Mean	Standard deviation	Minimum	Maximum
Lake [14]	Normal	0.035	0.065	-	-
Sea [14]	Normal	0.009	0.003	-	-
Terrestrial [15]	Uniform	0.46	-	0.03	0.96

As can be seen from the table above, only a small percentage of the C-14 in water bodies is assumed to be available for release to the atmosphere (< 3.5%), and less than half of the DIC in the soil pore water is assumed to be available for release to the atmosphere in the terrestrial ecosystem.

In the terrestrial ecosystem, a value of f_{H2CO3} towards the upper end of the distribution given in Table 13 would lead to a greater a proportion of the C-14 entering the soil entering the atmosphere, and then being lost from the system as a consequence of advective fluxes in the atmosphere. Calculated plant concentrations of C-14 would also be lower.

Piston velocity

The piston velocity (gas transfer velocity) is the height of the water that is equilibrated with the atmosphere per unit time for a given gas at a given temperature (m y^{-1}; see Section 8.8 of the Biosphere Parameters Report). There are several ways to define it, the majority of which are in some way dependent upon a study looking at releases of SF_6 from an oligotrophic lake (Cole and Caraco, 1998). The values assumed for the piston velocity in the SR-PSU assessment are given in Table 14 below. It is noted that the values assumed for the assessment are actually a factor of three lower than those calculated using the definition of piston velocity, as the original values were calculated based on open water and resulted in too great a degree of degassing from the soil. This adjustment of the piston velocity values, noted in Section 8.3.5 of the Biosphere FEP Handling Report as being “coarse”, is not well justified in the documentation.

[14] Data from April-November used

[15] pH range of 5 – 8 considered

Table 14: Distribution of piston velocity (m y^{-1}) assumed in the SR-PSU assessment. The values in brackets are those which were calculated, but ultimately rejected as they were deemed to lead to too high a release of C-14 from the soil or water body.

Ecosystem	Distribution	Mean / Central value	Standard deviation	Min	Max
Lake [16]	Normal	201	26	-	-
Sea [14]	Normal	187	26	-	-
Terrestrial – global warming base case[17]	Uniform	50 (151)	-	45 (145)	55 (157)
Terrestrial – periglacial climate case	Uniform	47 (141)	-	42 (133)	52 (152)
Terrestrial – extended global warming climate case	Uniform	46 (137)	-	41 (134)	51 (145)

It is noteworthy, that the parameterisation of degassing described above is relevant to aquatic ecosystems and terrestrial mire ecosystems only.

Degassing from agricultural soils

In all the agricultural ecosystems considered, degassing is assumed to be dependent on a parameter f_{gas}, which is calculated from the fraction of pore space filled with water and the solubility coefficient for CO_2 in pore water. In the definition of degassing for these ecosystems in the Biosphere Model Report, there is a scaling factor of 2 that appears in some, but not all of the equations used in their definition, and with no explanation as to its presence. In the infield-outland agriculture, this scaling factor appears both in the definition of the transfer rate (Equation 7-15) and also f_{gas} (Equation 7-16). It appears in the transfer rate for degassing from the drained mire cultivation system (Equation 7-39), which references back to Equation 7-16 for f_{gas}. However, for garden plot cultivation, the scaling factor appears only in the transfer rate definition (Equation 7-64) and not the definition of f_{gas} (Equation 7-65). The scaling factor of 2 does not appear in Equation B-6 of the Biosphere Model Report. In the Ecolego implementation of the model, the scaling factor of 2 appears only in the definition of the transfer fluxes, not in the definition of f_{gas}.

Calculated degassing rates

From the data provided in the Biosphere Parameter Report, and also data found in the Ecolego implementation of the biosphere model, it is possible to estimate the transfer rates (y^{-1}) associated with degassing from these various aquatic and terrestrial ecosystems (Table 15). Where there are biosphere object specific transfer rates, focus has been given to biosphere objects 157_1 and 157_2. It is noteworthy that the terrestrial degassing rates are all at least a factor of 5.8 higher than that suggested by Sheppard et al. (1991), 0.04 d^{-1}, which was based on field observations for high organic matter soils. That value was recommended by Sheppard et al. (2006) to be used as the geometric mean of a log-normal distribution with a GSD of 3.2. Oertel et al. (2016) presents measured soil emissions of both CO_2 and CH_4 in a range of soils, and climate zones. These demonstrate that there can be large variance in emission rates, though a conversion to a fractional rate was not undertaken to permit comparison with the values used in the SR-PSU assessment.

[16] Data from April-November used

[17] pH range of 5 – 8 considered

Table 15: Derived degassing rates (y^{-1}) based on information presented in SR-PSU documentation and the Ecolego implementation of the biosphere model

Ecosystem	Degassing rate (y^{-1})	Degassing rate (d^{-1})
Lake	19.5 [18]	~ 0.05
Sea	0.01 – 2.05 [19]	0.00003 – 0.01
Terrestrial - mire	85.2 [20]	0.23
Terrestrial – infield-outland agriculture	428.6	1.17
Terrestrial – drained mire system	~ 130	~ 0.36
Terrestrial – garden plot cultivation	428.6	1.17

3.4. Editorial Observations

On a general terminological theme, some of the descriptions of processes involving carbon in the SR-PSU documentation would have been less confusing if clearer definitions of the forms or carbon and organic matter had been given in the reports. For example:

- 'labile carbon' is sometimes referred to as 'non-decomposable' carbon and sometimes as 'non-refractory'; and
- 'refractory' (non-labile) carbon is specifically mentioned many times through the reports, but when describing soil organic matter compartments (e.g. RegoUp_org in section 7.1.1 of the Biosphere Model Report) 'refractory' carbon seems to be synonymous with 'soil organic matter' since all non-refractory or labile organic matter is considered to be decomposed on a time scale of less than one year.

Examination of the two descriptions of the atmospheric model show that the equations presented in Section 8 of Biosphere Model Report and Section 2 of Avila and Kovalets (2016) are almost entirely identical. However, there is a difference as to how the wind velocity in the canopy atmosphere is defined. It is defined in Equation 8-19 of Biosphere Model Report as follows:

$$Vel_{wind,CA} = Vel_{wind}(z_{CA})\frac{e^{-Coeff_{ext}}}{Coeff_{ext}} \quad (3)$$

In contrast, Equation 2-17 of Avila and Kovalets (2016) defines it as:

$$Vel_{wind,CA} = Vel_{wind}(z_{CA})\frac{1-e^{-Coeff_{ext}}}{Coeff_{ext}} \quad (4)$$

It is the equation as reported in Avila and Kovalets (2016) that has been implemented in the Ecolego model.

[18] Based on long term evolution of biosphere object 157_1
[19] Based on evolution of the sea in biosphere object 157_2.
[20] Based on biosphere object 157_2.

3.5. Conclusions of C-14 Review

The main conclusions drawn from review of the SR-PSU biosphere model for C-14 are summarised below.

Regolith

- Organic carbon pools have been explicitly introduced to improve the way that the carbon balance is represented.
- The existence and distinction in the behaviour of $^{14}CH_4$ in regolith layers, notably in the mire, is not discussed at all and is completely neglected in the biosphere modelling.

Aquatic ecosystem

- The assumed release to biosphere object 157_2, which does not have a water body, means that people are less exposed to contaminated fish (much of the C-14 degasses from the mire surface before reaching the lake that is present in Object 157-1), the consumption of which dominated the C-14 dose in the SAR-08 assessment.
- The modelling approach adopted for C-14 accumulation in fish results in significantly lower concentration ratios when compared against IAEA recommended values.

Terrestrial ecosystem

- The assumed degassing rates from soil are much higher than those used in other assessments. There is potential for further comparison of the rates against more recent literature sources.
- The assumed refractory organic matter content is lower than might be expected for mire vegetation such as *Spaghnum* moss. This leads to a greater proportion of decayed matter entering the soil pore water, for release to the atmosphere, than might be appropriate for such ecosystems

Atmospheric sub-model

- The new atmospheric exchange model provides an improved representation of micrometeorological processes. Similar models have been adopted by other waste management organisations in support of their safety assessments over recent years.

4. Review of K_d and CR

Sorption coefficients (K_d) and concentration ratios (CR) are key empirical parameters used in the SR-PSU biosphere model. Therefore, the traceability of these parameters, whether they originate from measurements taken by SKB at Forsmark or Laxemar, or whether they have been previously published by other authors, is of major importance. The site-specific K_d and CR values (i.e. from Forsmark and Laxemar) appear to originate from measurements taken as part of the SR-Site assessment and can ultimately be traced back to the SICADA database according to references made in the documents supplied to as part of this review (see below).

The initial review phase concluded with several questions to be addressed in the main review (SSM, 2016).

- For the literature sources of K_ds and CRs, what is the data overlap between IAEA (2010), ERICA and ICRP (2009)?
- How is the range in variability of K_d and CR translated within *plausible limits*?
- Are parameters for different elements really lumped together when determining plausible limits?
- How (and why) are CRs normalised with respect to carbon contents of organisms?

Finally, the major question, encompassing all the preceding questions, was:

- Is the SR-PSU K_d and CR data base and associated files (or a sub-set of these) available for scrutinyi?

The issue of literature data overlap is discussed further in Section 4.1. The methodology for determining plausible limits, including the aggregation of parameters for different elements, is reviewed in Section 4.2. The normalisation of CRs with respect to carbon contents of organisms is discussed in Section 4.3. SKB's methodology for calculating the distributions of K_d and CRs for the SR-PSU assessment is scrutinised in Section 4.4.

4.1. Degree of Overlap between Literature Sources of Kds and CRs

As described in Section 4.5 of the K_d and CR Report, comparisons have been made between site data based distributions of K_d and CR and literature data. In particular, some or all of the following five comparisons have been made for each parameter, depending on the number of datasets available.

1. Literature distribution (min and max) vs. Forsmark distribution (5% and 95% of distribution with "plausible" GSD).
2. Literature distribution (min and max) vs. Laxemar distribution (5% and 95% of distribution with "plausible" GSD).
3. Literature distribution (min and max) vs. combined Forsmark and Laxemar distribution (5% and 95% of distribution with "plausible" GSD).
4. Forsmark distribution vs. Laxemar distribution (both 5% and 95% of distribution with "plausible" GSD).
5. Multiple literature distributions, compared pairwise (min and max).

In the majority of instances where there are multiple literature sources, then the distributions overlap. There are some notable exceptions[21], which are summarised below.

With respect to K_ds for organic soils (kd_regoPeat, kd_regoUp_drain and kd_regoUp_ter), two literature sources have been used. These are both from IAEA (2010), but the data relating to "organic soils" and the data relating to "all soils" are considered as separate sources. Given the latter category will encompass a number of mineral soil samples, it is perhaps not surprising that there is a lack of overlap in the K_d distributions for almost half of the radionuclides considered in the SR-PSU assessment: Ac, Ag, Bi, Ca, Ho, Nb, Pa, Pd, Po, Ra, Se, Sm, Sn and Zr.

With respect to the CRs for cereals, vegetables and tubers, literature data for these all come from IAEA (2010), although multiple plant types are used for each. For example, data relating to tubers (all soils) and root vegetables (all soils) from IAEA (2010) have been used to look at cR_agri_tuber, with differences between the distributions of those for Ba, Nb, Tc and Zr.

There are many differences in the distributions reported in ICRP (2011), ERICA and IAEA (2010) for non-human biota, although typically only a small subset of elements has data from more than one literature source for each CR being considered.

When both site and literature data are available, there are several instances where there is little if any overlap between the distribution of site data and distributions from the literature data.

One such is example is Kd_regoGL for Ni, Ca, Cs, Ho, Nb and Sm (see Section 5.2 of the K_d and CR report). The value for Ni used in the SR-PSU assessment is based on data for Zn, which is used as an element analogue for this parameter. SKB suggest that this discrepancy might be explained by the larger specific surface area of the clay particles included in the glacial clay samples and that literature data probably represent more coarse soils than glacial clay. As the glacial clay soil is assumed to become mixed with agricultural soil following drainage of the mire, this high level of retention leads to an increased amount of Ni being available for plant uptake, and thus a greater amount to be taken up by cattle grazing in the area.

4.2. Plausible Parameter Variation

Having calculated K_ds and CRs from site-specific data from Forsmark and Laxemar, geometric means (GMs) and geometric standard deviations (GSDs) are established. Literature values of K_ds and CRs, also entered into the 'K_d/CR compilation' database, are used to evaluate the 'plausibility' of the GSDs derived from site-specific data. Consideration is given here to that methodology, using kd_PM_lake and kd_PM_sea as a worked example to understand and demonstrate the methodology as described in Section 4.3 of the K_d and CR Report. These two parameters have been chosen because they represent the smallest collation of parameters used to define one of the "*plausible parameter variation*" distributions for GSD.

[21] There are further disagreements between literature sources which are indicated in the Kd and CR Report but are not mentioned below.

The 'plausibility' of the GSD derived from the site-specific data is based upon two primary factors. The first factor is the number of N of site data derived values for a given element for a particular K_d or CR. The second factor is the cumulative distribution of GSDs obtained from site specific data for that K_d or CR parameter, and similar K_ds or CRs, across all elements.

With respect to kd_PM_lake, there are site data to support the parameterisation of 62 elements, with between one to six data points per element. There are 554 paired samples in total, across all elements. With respect to kd_PM_sea, there are site data to support the parameterisation of 63 elements, with between one to eight data points per element. There are 381 paired samples in total, across all elements. As noted in Section 4.3 of K_d and CR Report, data from all elements were included in the analysis of GSD variation, not just the elements included in SR-PSU[22].

According to Table 4-3 of the K_d and CR Report the average of the 5th, 50th and 95th percentiles of the cumulative distribution of GSD of kd_PM_sea and kd_PM_lake are then used to define a more generic definition of GSD across kd_PM in both types of water body. From Table 16 it is clear that the GSD distribution derived from the data used in this review (the Forsmark data) differs from that presented in the SR-PSU assessment. Those three percentiles are then rounded up to the nearest integer to define what are termed as GSDmin, GSDmean and GSDmax.

Table 16: Distribution of GSD for kd_PM.

Kd_PM_x	5%	50%	95%
Kd_PM (from Table 4-3 of Trojbom et al., 2013)	1.5	2.2	7.1
kd_PM_lake (review)	1.4	2.0	3.6
kd_PM_sea (review)	1.3	2.1	8.8
kd_PM (review)	1.3	2.1	5.7

The degree of confidence placed in the estimate of GSD for a specific element and a particular K_d or CR parameter is then evaluated based on N, the lowest number of the two sets of data required to calculate that parameter. In Section 4.4.2 of the K_d and CR Report, SKB acknowledge that the chosen N limits are arbitrarily and mainly set to give a reasonable division of (the site) data. For low N (< 3), SKB consider that the variability is such that the GSD should be at least as large as GSDmax, i.e. the upper end of GSD across all elements for that particular K_d or CR parameter. This presumably is to acknowledge that the site data may have missed some tails of the distribution due to the limited number of samples. For intermediate N (3 <= N < 10), SKB assume that the GSD for that particular element should be at least GSDmean. Finally, for high N (> 10), SKB assume that GSD should be at least GSDmin. For K_d, N never exceeds 11, and for the majority of elements across all ten K_ds N is less than 10. With respect to CR, the majority of site based N are less than 20. Higher values of N (over 100) are only ever associated with literature sources, and therefore were not included in any form of "plausible limits" analysis.

Examples of the implications of SKB's judgement on distributions are given in Table 17 and Table 18 below, for kd_PM_sea and kd_PM_lake respectively. In the GSD columns, the number in brackets is the GSD imposed upon that element based on "plausible variation". In some instances, the enforcement of a GSD based on the

[22] Of those 60+ elements for which there is site data from Forsmark, only 18 are included in the SR-PSU assessment.

behaviour of all elements for kd_PM leads to an almost doubling of the GSD than if using the element and water type specific site measurements.

Only for two of the element-K_d combinations in the below tables is there anything more than a single literature value available (as reported by SKB). These are kd_PM_lake[Cs] and kd_PM_lake[I]. For Cs, IAEA (2010) gives a geometric mean value of 2.9E+1 m^3 kg^{-1} dw, with a GSD of 5.9, based on 219 field measurements. For I, IAEA (2010) report a geometric mean value of 4.4E0 m^3 kg^{-1} dw, with a GSD of 14, based on 124 laboratory adsorption experiments (in oxic conditions). Figure 15 shows the 5th to 95th percentile ranges for these parameter distributions, based on the SR-PSU site data and also the IAEA (2010) data; the 5th and 95th percentiles are the points SKB used to compare distributions (see Section 4.5 of K_d and CR Report).

In addition, data relating to U are available from a single publication (Onishi et al., 1991), which were later reported in IAEA (1994). They report a range of 1.0E-2 to 7.0E+1 m^3 kg^{-1} dw for the K_d of U in aqueous systems, with an expected value of 5.0E-2 m^3 kg^{-1} dw. Note that IAEA (2010) states the U data should be used with caution, because of the single source.

Table 17: kd_PM_sea (m^3 kg^{-1}) distributions for selected elements

	SR-PSU			Review		
Element	N	GM	GSD[23]	N	GM	GSD
Ac [24]	5	4.6E+02	(3)	-	-	-
Ca	8	2.8E-01	9.8	8	2.8E-01	8.5
Cl	1	6.4E-04	(5)	1	6.4E-04	-
Cs	5	1.9E+01	4.0	5	1.9E+01	3.4
I	5	5.3E+00	1.8 (3)	5	5.3E+00	1.7
Mo	8	2.3E+00	10.2	8	2.3E+00	8.8
Ni	8	1.4E+01	1.3 (3)	8	1.4E+01	1.3
U	5	1.2E+00	2.1 (3)	5	1.2E+00	1.9

[23] The number in brackets is the GSD imposed upon that element based on "plausible variation"
[24] Site data for Sm has been used by SKB as an element analogue for Ac. For this reason, no review comparison has been made.

Table 18: kd_PM_lake (m^3 kg^{-1}) distributions for selected elements

	SR-PSU			Review		
Element	N	GM	GSD[23]	N	GM	GSD
Ac [24]	6	9.1E+01	(3)	-	-	-
Ca	6	1.1E+00	2.0 (3)	6	1.1E+00	1.9
Cl [25]	6	2.3E+00	4.0	-	-	-
Cs	6	1.0E+02	2.8 (3)	6	1.0E+02	2.6
I	5	1.6E+01	2.0 (3)	5	1.6E+01	1.8
Mo	6	1.2E+01	1.4 (3)	6	1.2E+01	1.4
Ni	6	2.8E+01	2.1 (3)	6	2.8E+01	2.0
U	6	8.4E+00	6.9	6	8.4E+00	5.8

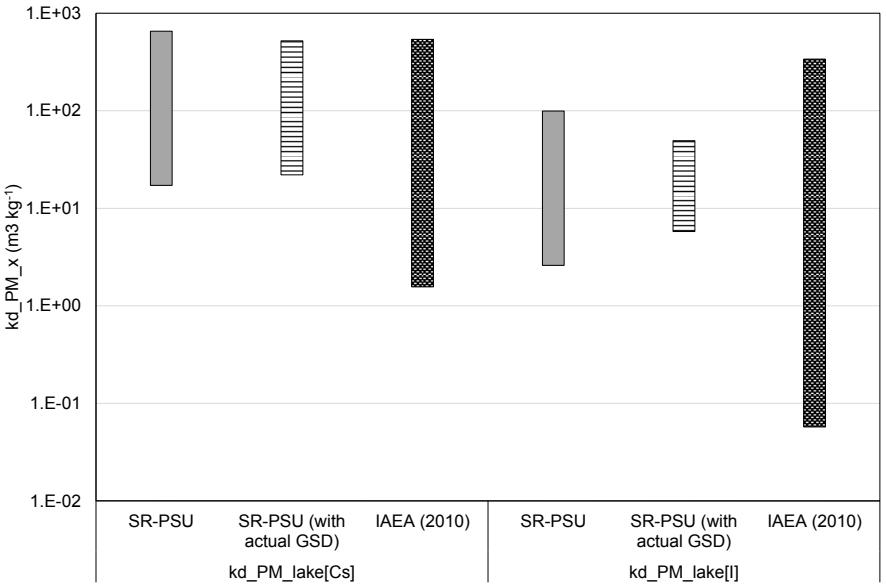

Figure 15: 5th to 95th percentile ranges of kd_PM_lake[Cs] and kd_PM_lake[I] based on three different distributions: SR-PSU (with the GSD based on "plausible variation"), SR-PSU (with the GSD based on the data for that element and parameter), and IAEA (2010).

4.3. Normalisation of CRs with respect to Carbon Contents of Organisms

According to the Biosphere Parameter Report and the K_d and CR Report, where site specific data are available, these have been used to convert concentration ratios defined in terms of the dry weight of the organism to mass of carbon. From examination of cR_agri_Cereal for Mo, it is clear that this is done on a sample by sample basis for the organisms, converting their content of a given element on a dry

[25] Site data for Br has been used by SKB as an element analogue for Cl. For this reason, no review comparison has been made.

weight basis to that of a kgC basis, before combining the data with the soil or water elemental content data to derive the CR values.

The use of sample-specific carbon content data to convert concentration ratios from a fresh or dry weight basis to a per mass of carbon basis is appropriate, but means that the parameters used by SKB in this assessment are less tractable than if literature values of carbon contents for biota were used.

4.4. K_d and CR Parameterisation

Following the initial review phase, SKB made two Microsoft Access database files and several supporting files available. The data files were accompanied by two document files:

- Grolander and Tröjbom (2016a) - Guide to the implementation of the SR-PSU K_d and CR parameterisation in two Access databases (referred to below as 'the Guide'); and
- Grolander and Tröjbom (2016b) - Manual reproduction of parameter values in SR-PSU (referred to below as 'the Manual Guide').

The first of these documents provides an extremely detailed description of the operation of the two databases, specifically the automated generation of the 2,139 K_d and CR values which are 'delivered' to the dose assessment model described in the Biosphere Model Report.

The automated derivation of the K_d and CR database (called the "*K_d/CR data compilation*") involves numerous steps, including the generation of intermediate files, which are undertaken using a large number of Access database queries and bespoke Visual Basic functions. The processes involved are fully described in the first of the above documents – these are reviewed and commented on in Section 4.4.1. The overall automated process within and around the two databases is so complex, however, that the authors have also provided the second document, which describes the calculation and final selection of K_d and CR values manually. This process is reviewed in Section 4.4.2. Finally, some example parameter distributions have been calculated using SKB's methodology as part of the review, and are presented in Section 4.5.

4.4.1. Guide to the implementation of the SR-PSU K_d and CR parameterisation in two Access databases

Figure 16 is provided to summarise the key data files provided by SKB and the interrelationships between these files. At the centre of the file collection are two Access databases, which are named:

- SKB_Chemistry_SR_PSU.accdb
- SKB_Kd_CR_131115.accdb

The aim of the database operations described by Grolander and Tröjbom (2016a) is to produce a logically-reasoned and quality-assured collection of relevant K_d and CR values that can then be used in the SR-PSU biosphere calculations. This final collection of parameter values is referred to as the "K_d/CR data compilation" which is actually a table within the Access database file SKB_Kd_CR_131115. This Access table is named "FinalTable" and represents the end-point of the process,

though can be subject to iterative review and update as indicated at the bottom of Figure 16.

The starting point is the 'root' database for these site-specific data in the form of an Excel workbook SKB_Chemistry_SR_PSU, containing elemental concentrations in biota, waters and soils obtained by SKB at Forsmark and Laxemar. These appear to originate from measurements taken as part of the SR-Site assessment and can ultimately be traced back to the SICADA database. They are described as "*quality-controlled data on element concentrations in water, regolith and biota*" (Section 2.1.1 of the Guide). The Excel file provides either an extract of this database or it represents the full collection of site-specific measurements available to SKB, from which site-specific K_d and CR values can be calculated for Forsmark and Laxemar. The key worksheets within the Excel workbook are 'Data Water' (holding 8,150 records on water chemistry and associated information) and 'Data Regolith and Biota' (holding 749 records on chemistry plus associated information).

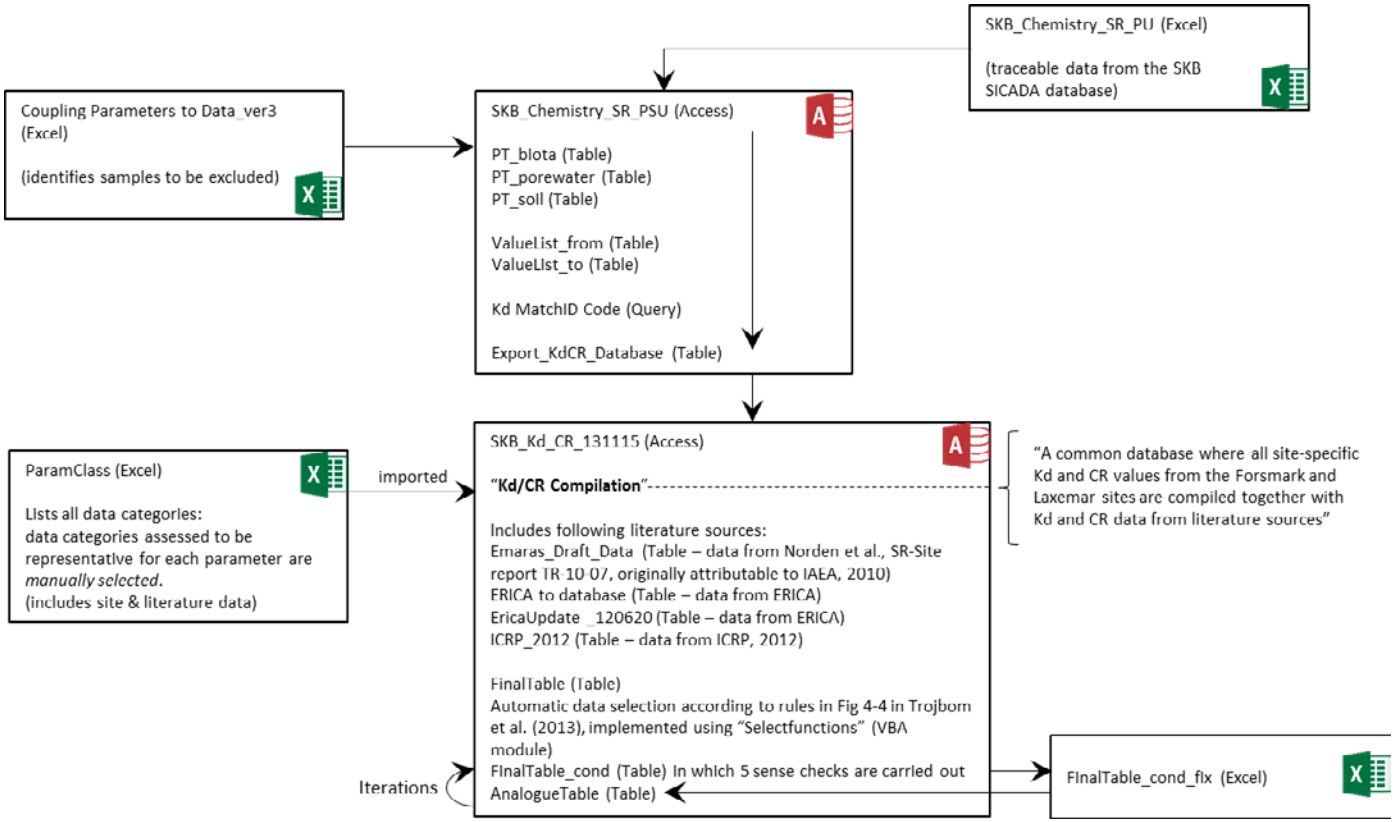

Figure 16: Graphical summary of SR-PSU K_d and CR parameterisation process based on 2 Access databases. For the sake of traceability, a full directory address of the 'chemistry' database within SKB's SR-PSU repository is provided: (svn://svn.skb.se/projekt/SFR/SR-PSU/Indata/Chemistry/SKB_Chemistry_SR_PSU.accdb).

As indicated in Figure 16, the fundamental chemistry data in Excel file SKB_Chemistry_SR_PSU are imported into the first Access database SKB_Chemistry_SR_PSU. After import, these data reside in two Access data tables:

- Regolith&Biota (749 records)
- Water (8,150 records)

which equate to the two key worksheets in the original Excel file. Additional tables within the Access database which appear to hold data on soil, water and biota chemistry are:

- PT_biota (10,197 records)
- PT_porewater (2,057 records)
- PT_soil (2,231 records)

Although the numbers of records in these additional Access data tables are greater than those in the corresponding Excel tables it is not clear whether the 'root' data from Excel workbook SKB_Chemistry_SR_PSU have been supplemented with additional elemental concentration values at some stage, although some mention is made of this in Section 2.2.1 of the Guide (Appendix A – "*data files originally assembled for the previous safety assessment SR-Site, combined with recent data from SICADA*"). The original locations of the Regolith&Biota and Water data tables are given within the SR-PSU SVN (Table 2-1, Appendix A).

Taken overall, the stated aim of the automated parameterisation process is to "*compare(s) and select(s) data from different sources in order to achieve an as coherent dataset as possible*". Both Access data bases (SKB_Chemistry_SR_PSU and SKB_Kd_CR_131115) are involved in this process, which is highly automated. This, apparently, is necessary because of the complexity of the data sources and their interrelationships. This complexity is never explicitly stated, but the coordinated use of the databases "*to handle the vast number of data in an efficient and rational way*" (Section 1 of the Guide) gives an indication of the difficulty of the task of making sense of SKB's site-specific data. Notwithstanding the highly automated approach to parameter calculation and selection, the authors also state that "*the parameterisation process contains subjective steps in the form of manual considerations and judgements*".

The overall process of selecting appropriate K_d and CR values for use in the SR-PSU biosphere calculations is broken down into two major parts:

1. Generation of the K_d/CR data compilation, which is carried out in two steps:
   - Calculation of site-specific K_d and CR values (described in Section 2.1 of the Guide); and
   - Compilation of data from available literature sources stored in Access database SKB_Kd_CR_131115) (described in Section 2.2 of the Guide).
2. Evaluation and selection of data from the K_d/CR compilation and adjustments of the final parameter values (implemented in Access database SKB_Kd_CR_131115).

As described above and summarised in Figure 16, several files are used in the implementation of the two-stage process to calculate and select the 2,139 unique K_d and CR parameters delivered to the dose assessment model in SR-PSU. These files

are all identified in Table 1-1 of the Guide and all were present in the files available for this review.

Table 1-2 of the Guide lists the K_d and CR parameters actually needed for the SR-PSU assessment. These consist of 18 freshwater CRs, 16 marine CRs, four agricultural CRs, 18 terrestrial CRs, 11 K_ds and two agricultural transfer coefficients. Each of these parameters is estimated for 31 elements and values for each of these parameter/element combinations are derived from a variety of sources. The 'best' values can be considered to be site-specific, but for some groupings of parameters the site-specific values were sparse.

As an example, the numbers of "site" values for freshwater CR's are as follows:

- CR Lake Bivalve NHB – 20
- CR Lake Fish – 15
- CR Lake Fish NHB – 15
- CR Lake Macro – 19

This gives a total of 69 site-specific values from a total CR Lake of 18 x 31 = 558. Thus, only 12.4% of the freshwater lake CR's are based on site data. Turning attention to K_ds (341 values in total), most values appear to be derived from site-specific data, although Kds for some elements are derived solely from element analogues (Ac, Am, Cm, Np, Pa, Po, Pu and Tc). In the case of Tc, an artificial radionuclide, this is understandable since is likely to be effectively absent at any measurable values at the study sites.

The calculation of site-specific K_d and CR values is carried out in five steps.

STEP 1
The parameters are coupled to suitable categories of site-specific concentration data in an Excel file (Coupling parameters to data_ver3.xlsx) (see Figure 16).
This Excel workbook consists of separate worksheets for biota, regolith and water. E.g. for 'regolith', there are 218 records for terrestrial, limnic and marine samples taken from Laxemar (Simpevarp) and Forsmark, with descriptions of sample type and sub-type, how they were prepared for analysis and references to the 11 SKB reports from which the data have been derived (a mixture of P, R and TR reports) (curiously, 12 records are simply referenced as 'n').

STEP 2
Each data worksheet within the 'Coupling parameters to data_ver3' workbook is accompanied by a 'Details' worksheet in which samples to be excluded have been filtered manually (highlighted in red in the appropriate worksheet). For example, in the Regolith ('Details_soil' worksheet) 27 records have been highlighted as being excluded for a variety of reasons including: "*duplicate samples, spiked samples?, duplicate – identical samples*". Interestingly all the 'spiked' samples were from a single SKB report (Sheppard et al., 2009).

Reasons for excluding biota samples include "*Probable mineral contaminated sample!"*. Selected water samples are excluded because *"The concentrations differ, these samples are coupled to suspended matter samples*".

STEP 3
Information in the 'Coupling parameters to data_ver3' spreadsheet is imported to SKB_Chemistry_SR_PSU Access data base, as illustrated in Figure 16. As described above, the "quality controlled data on element concentrations in water,

regolith and biota from both Forsmark (FM) and Laxemar (LX)" are held within two tables within the database, namely:

- Regolith&Biota
- Water

Each with different numbers of records. Checking the Regolith&Biota table, data from the 'excluded' Sheppard et al. (2009) report are still included in the database – it is not clear whether they should have been excluded *before* import into the Access database, or whether they are simply ignored in the calculation of K_ds.

STEP 4

In the fourth step in the automated calculation of site-specific K_d and CR values, two macros ('skapa_ValueList_to' and 'skapa_ValueList_from'[26]), and the numerous queries they invoke, create the following two tables within the SKB_Chemistry_SR_PSU Access data base (see Figure 16):

- ValueList_to
- ValueList_from

The tables represent the numerators and denominators, respectively, in the K_d and CR calculations. Therefore, the purpose of the two macros is evidently to select 'matched' samples from which appropriate ratios can be calculated.

As a check on the data within the ValueList_to and ValueList_from tables, SKB Sample No 23021 was used as an example:

- both tables were filtered for SKB Sample No 23021
- 354 concentration values from 'ValueList_from', 318 of which had concentrations > 0 (i.e. were useable in ratio calculations)
- 59 concentration values from 'ValueList_to', 53 of which had concentrations > 0 (i.e. were useable in ratio calculations) (solution data - NO)

It is not immediately clear which of these tables is used to calculate what. The last column in each table is a 'From' or 'To' parameter and it is apparent that the same data can be used in each of these columns – i.e. soil concentration of an element is a 'From' parameter when calculating CR to plants, but is a 'To' parameter when calculating a regolith K_d.

As indicted in Figure 16, the Access database query 'Kd_match_idcode' is used to select appropriate data pairs from the same geographical location (IDCODE) and the same sample depth (SECUP) (the structure of this query is shown in Figure 2-1 of the Guide). If more than one measurement has been taken at the same location and depth this can lead to multiple combinations of solid and liquid data which, presumably, is why one of the reasons for excluding data in Step 2 of the calculation is to eliminate "duplicate-identical samples". In the example provided for Ni Kd_regoLow, it is stated that:

> *"Since the analytical replicates were omitted prior to the matching the actual pairs formed therefore represent unique sampling occasions at specific locations and depth. From the query expression could be concluded that if there are more than one sample representing the same IDCODE and SECUP, data pairs will be formed for all possible permutations of the samples with identical IDCODE and SECUP combinations. In the SR-PSU*

[26] 'Skapa' translates to English as 'create'.

parameterisation this only occurred for one sample where two different digestions methods were used to measure the sorbed fraction of the marine sediment sample PFM006045 (SKB sample no 23546 and 23548).” (p. 10, para 1 of the Guide).

STEP 5

The final step in site-specific K_d and CR calculation uses appropriate data pairs, taken from the ValueList_to and ValueList_from tables, to calculate CRs and K_ds which are then stored in the Access table ‘Export_KdCR_database’ (see Figure 16). This table contains 8336 records which can be broken down into 1958 Kds, 1928 CR_s (terrestrial biota), 620 CR_b (food to biota), 3830 CR_w (aquatic biota).

Applying a filter for Kd_regoLow values for Ni gives two lines in the database, one for Forsmark only data (FM), the other for Forsmark and Laxemar combined (F&L); see Table 19.

Table 19: Results for site-specific calculation of Kd_regoLow for nickel taken from the Access table ‘Export_KdCR_database’.

Site	Forsmark	Forsmark and Laxemar
N	7	7
N_from	7	7
N_to	7	7
MinV	0.6187	0.6187
GM	0.7924	0.7924
MaxV	1.6298	1.6298
GSD	1.4308	1.4308
Unit	m3/kgdw	m3/kgdw
ParameterDB	Kd	Kd
Reference	PSUprel_FM	PSUprel_F&L

Having examined the ‘Export_KdCR_database’ table it is evident that it does not contain individual replicate values for K_ds and CRs, but contains the final geometric means (GM), geometric standard deviations (GSD), minima and maxima for each parameter. It is stated in Section 2.1.1 of the Guide that the query ‘Kd_match_idcode’ is “*where the statistics are calculated*” prior to the deposition of these statistics in stored in the Access table ‘Export_KdCR_database’. Further examination reveals that the query ‘Kd_match_idcode_persample’ can be used to interrogate the database for individual replicate values of each combination of element and parameter (as illustrated in Table 2-3 in ‘the Guide’).

The operation of the macros in the sequence of data handling steps is complex and a little unclear, even though they are obviously ‘effective’ as demonstrated by the ‘worked’ examples provided for:

- Kd_regoLow for nickel
- CR_LakeFish for neptunium
- CR_AgriVeg for caesium

The first of these examples has been checked through against the data table and screenshots of queries provided in Section 2.1.1 of the Guide and found to agree with the description and example figures and data. Overall, the process of calculating the site-specific K_d and CR values is highly complex but, ultimately, a traceable procedure. However, there is a danger is that the database and spreadsheet

operations are so complex that it is easy to lose sight of the importance of the parameter values produced. Despite the sophistication of the data structures and the automated routines that link them, the eventual statistical power of the parameters obtained is limited by low numbers of data pairs from which K_ds and CRs can ultimately be calculated (e.g. N=7 for Kd RegoLow for nickel).

A key operation is the estimation of what the authors call 'plausible parameter variation', which is based on site-specific data from Forsmark and Laxemar. The variation of parameter values for individual elements is judged against the overall variation for ALL elements within SKB's chemistry database, even those that are not included in the SR-PSU calculations. It is stated by K_d and CR Report that, by using this method, "*it is assumed that the overall range of the GSD variation in a parameter group is better captured*". However, it is difficult to see how the statistical variation of an element with a specific set of chemical characteristics should be better represented by the variation in a range of elements of substantially different chemistry. The decision to implement this method seems arbitrary and may reflect the low statistical power (low N) of the site-specific parameter values available to SKB.

The implementation of the complex series of steps in determining plausible parameter variation (originally described by K_d and CR Report, section 4.4) is achieved using a series of Visual Basic functions within VBA module "SelectFunctions", presented in Appendix A of the Guide.

Having calculated site-specific K_ds and CRs with plausible GSDs, operations move to the second Access database (SKB_Kd_CR_131115) in which literature data are compiled in the following Access tables:

- Emaras_Draft_Data (data from Norden et al., SR-Site report TR-10-07, originally attributable to IAEA, 2010)
- ERICA to database (data from ERICA)
- EricaUpdate _120620 (data from ERICA)
- ICRP_2012 (data from ICRP, 2012)

The final selection of appropriate K_d and CR values for use in the SR-PSU assessment is achieved by comparing site-specific parameter values (with 'plausible' GSDs) with available literature data. This is achieved in a separate Excel worksheet named 'ParamClass' (see Figure 16). The operation of this part of the process is illustrated with screen shots in Figures 3-1 to 3-3 of the Guide which show the data categories assigned to each parameter class for Kd_regolow, CR Lake_fish and CR Agri_veg, respectively. These figures illustrate the ranking of literature sources from L1 to L5, of which L1 represents the most appropriate literature data for the parameter being considered.

Once again, the selection of the most appropriate values is highly automated using a VBA script described in the Appendix of the Guide, following the series of rules described by Tröjbom et al. (2013, section 4.4.2). The literature sources are used as one of the 'sense checks' for site-specific K_ds and CRs, by comparing geometric means, geometric standard deviations, maximum and minimum values between the former and the latter. Although the automated 'sense checks', clearly work correctly, they are somewhat difficult to follow. In contrast, this process of checking site-specific versus literature values is quite well explained, with the aid of graphs, in the Manual Guide, as described in Section 4.4.2, below.

Finally, the parameters are selected in Excel workbook 'FinalTable_cond_fix' (Figure 16) which can be iteratively updated via Access table AnalogueTable in 'SKB_Kd_CR_131115'. This provides the facility to "*override the initial selection of data by importing the information back into the Access database*".

The final selection of parameter values can be viewed in Excel workbook 'FinalTable_cond_fix' which represents the endpoint of the parameter selection process. Usefully, the version of this workbook supplied to us (FinalTable_cond_fix_PLOTB) contains several summary graphs of the CRs and Kds, with geometric means, maxima and minima plotted for visual comparison.

4.4.2. Manual reproduction of K_d and CR parameter values

Given the complexity of the automated parameter selection and screening procedures described above, SKB have provided several worked examples that can be implemented manually, without the need to "*understand the details of the databases*". These manual operations are described in 'the Manual Guide'.

As with the automated parameter selection process, the overall manual process involves:

- calculation of site-specific K_d and CR values; and
- final data evaluation and selection from all available data sources (site-specific and literature).

A collection of data files necessary for the manual calculation and selection procedures have been provided. Elemental concentrations in relevant media from the Forsmark and Laxemar sites are made available in the same Excel workbook which provides the basis for the automated site-specific calculations described above:

- SKB_Chemistry_SR_PSU.xlsx

This is "*based on traceable data from the SKB SICADA database*"[27], so should provide a direct link to the 'root' data sources for the SR-PSU assessment (and the SR-Site assessment prior to SR-PSU).

A key file in the manual calculation is the Excel workbook 'MATCHED_SNO.xlsx' which provides the identification numbers for appropriately matched pairs of samples for the calculation of K_ds and CRs. Usefully, the columns in the worksheet are labelled 'numerator' and 'denominator' to aid traceability. The K_d and CR calculations differ, however, in that K_ds are based on "*true sample pairs*" and the "*population statistics are based on these pairs, either per site or both sites (i.e. Forsmark and Laxemar) in combination*". For CRs, "*all possible permutations per site*" of elemental concentrations in soil or water (for terrestrial or aquatic organisms) with biota are used to calculate the ratio. This approach was adopted because the biota and environmental media were only occasionally sampled at the same locations or at the same times. "*N is defined by the lowest number of unique samples from either the numerator or the denominator of the selected samples*" (Section 2 of the Manual Guide).

[27] NB. this is mentioned on p. 3 of the Manual Guide report, nowhere else in the report.

Examples of manual calculations are provided for elements identified as being significant in our initial review – namely Ni, I, Ca, Mo and U – for the following parameters:

- Kd_regoLow
- CR_lake fish

For Kd_regoLow for Ni, individual soil and porewater concentrations for the sample pairs identified in 'MATCHED_SNO.xlsx' were checked against the 'root' database 'SKB_Chemistry_SR_PSU' and found to be correct, giving confidence in the descriptions provided.

The seven individual data pairs are shown in Table 2-2 in the Manual Guide, along with the 'summary' data (GM, GSD, minimum and maximum values) which are shown in Table 20, below.

Table 20: Results for manual calculation of Kd RegoLow for nickel as shown in Table 2-2 in the 'Manual Guide'.

Site	Forsmark
N	7
MinV	0.62
GM	0.79
MaxV	1.6
GSD	1.4
Unit	m3/kgdw

These are identical to the equivalent summary values obtained during the automated process from the Access table 'Export_KdCR_database', shown in Table 19 above, which gives confidence in the compatibility of both the automated and manual calculation processes. Examples are also provided for the manual calculation of Kd_regoLow for iodine, calcium, molybdenum and uranium. Each of the summary values presented in sections 2.1.2 to 2.1.5 in the Manual Guide has been checked against the results produced by the automated calculations and each was found to be in agreement.

Checking the examples provided for the manual calculation of CRs for lake fish, it is evident that the numbers of paired elemental concentrations for fish and lake water are much greater than for soils (N=48 for Forsmark and N=18 for Laxemar-Simpevarp). This arises, however, because the combination of "*all possible permutations*" is allowed for CRs. The ultimate value N for Lake Fish CRs is limited by both the "*lowest number of unique samples*" for either fish or water, and/or by the availability of elemental measurements above detection limit. An example is the CR value for nickel which, due to the fact that only one sample of fish muscle had a nickel concentration above the detection limit, N=1 for this element (Table 2-11 in the Manual Guide). Such data constraints obviously limit the statistical power of some of the site-specific parameters and make the selection of literature data necessary.

The second part of the manual calculation (starting at p. 31 in the Manual Guide) involves the evaluation of the site-specific K_ds and CRs and selection of the most appropriate data sources for inclusion in the final table. In many respects this is the most challenging part of the review and the manual calculations provide considerable help in working through the process.

Having calculated site-specific GMs and GSDs for K_ds and CRs, the next task is to compare the ranges with those of the published sources compiled within the Access database 'SKB_Kd_CR_131115'. This is referred to as the 'sense check'. In the case of K_ds this check is restricted to comparing the site-specific GSDs with the ranges of K_d provided by IAEA (2010), since this is the only literature source of K_ds. N.B. for the K_d manual calculation examples, each one has the statement "*no other **sense check** could be done since no other data sources are available*".

The limits of GSDs are presented in Table 4-2 of the K_d and CR Report (one slight error in the Manual Guide is the reference to Table 4-3 in the K_d and CR Report, which presumably means Table 4-2, since there is no Table 4-3). It is evident that the GSD limits in this table are the same for all elements in a given compartment – because they are based on observed GSDs for all elements for each parameter, as explained in the legend to Table 4-2 (Tröjbom et al, 2013). It is stated in the K_d and CR Report that "*that the procedure of defining these limits is to some extent subjective and based on the general assumption that it is conservative to widen the PDFs of selected parameter data*". This certainly a cautious 'empirical' approach, but the use of GSDs based on all elements is a curious approach given the statement that "*The GSD is expected to varies (sic.) between elements or element groups …*". With reference to Q-Q plots[28] in Figure 4-3 of the K_d and CR Report "*it can be concluded that the shape of the GSD distributions are skewed and varies greatly depending on the parameter. Consequently, no general assumptions of the nature of the GSD distributions can be made; therefore, the plausible limits for the GSD are defined as percentiles of the empirical distribution of the GSD for each parameter*".

The definitions of plausible limits for GSD are given on p. 44 of the K_d and CR Report:

- GSDmin denotes the lowest reasonable GSD expected for a parameter group;
- GSDmax is the highest expected GSD;
- GSDmean could be interpreted as the best estimate of the GSD for a parameter group;
- GSDmin and GSDmax are estimated from the 5th and 95th percentiles, respectively, of the observed GSD distribution of a parameter group; and
- GSDmean is based on the median of the GSD distribution of each parameter group.

Using Kd_regoLow for nickel as an example, the site-specific values are 'sense-checked' against Kds for 'All Soils' obtained from IAEA (2010). According to the definitions above, the GSDmin and GSDmax for the IAEA Kds for Ni can be calculated as the 5th and 95th percentiles, based on the GM and GSD given for Ni in 'All Soils' in IAEA (2010). These limits are provided in Table 3-1 of the Manual Guide and are 0.011 and 6.88 (GM = 0.28). Since the site-specific GSDmin (0.44) and GSDmax (1.43) lie within the IAEA (2010) range, the site data are considered to be "*suitable for the parameterisation*". In circumstances where the overlap between site-specific data and literature data is only partially available, if at all, then SKB recommend caution be exercised in using the site specific parameter values[29]. The parameter values are selected manually in such circumstances, with the justifications for the parameter values selected noted in the tables in the K_d and CR Report.

[28] Quantile-Quantile plots.
[29] Section 4.5.1 of the Kd and CR Report.

However, the final step is to set 'plausible limits' on the GSD range for each parameter. In the case of Kd RegoLow for Ni, the GSD limits in Table 4-2 of the K_d and CR Report are applied. Since the GSD limit in this table (3, based on all elements for the sake of pessimism) is greater than the empirically calculated site-specific GSD of 1.4, the larger GSD limit is adopted and the minimum and maximum values of the Ni K_d calculated as 5th and 95th percentiles based on the 'plausible' GSD and the site-specific GM. These final selected values are shown in Table 3-2 of the Manual Guide, as reproduced in Table 21 below.

Table 21: Final selected values for Kd RegoLow for nickel as shown in Table 3-2 in the Manual Guide.

Site	Forsmark
N	7
GM	0.79
GSD	3
Minimum	0.13
Maximum	4.82
Distribution	Log-normal
Unit	m3/kgdw

The other manually-calculated examples given for Kd_regoLow are for iodine, calcium, molybdenum and uranium. The GM and GSD values for each of these elements given in IAEA (2010) were all checked and found to be correct, so the 'sense checks' using these data sources are all taken to be accurate and reasonable. Reading through these examples, however, it is evident that for each element N=7 for Kd_regoLow, which reflects the fact that the original measurements of elemental concentrations were carried out in the same paired soil and pore water samples, which underlines the basic limitation of the site-specific parameter values which are restricted to low replication. This compares with generally much larger values of N for K_d values in the IAEA (2010) compilation though, as stated above, the sense-checks of SKB's Kds rely entirely on this single published database.

It is certainly more straightforward to follow through the whole process of calculating site-specific K_ds and CRs, the 'sense-checking' of these values with respect to published literature sources, and the final setting of plausible minima and maxima when this complex process is applied in the examples provided in the Manual Guide.

4.5. Example calculations of K_d and CR values

4.5.1. Rederivation of cR_agri_Cereal for Mo

Appendix F of the Radionuclide Transport Report notes cR_agri_Cereal as being one of the three key parameters in the sensitivity analysis with respect to the calculated human dose from Mo-93 exposure.

Table 6-18 of the K_d and CR Report states that 28 soil and 10 cereal samples collected from Forsmark were used to calculate this parameter value. The cereal data, which comes from Sheppard et al. (2011), comprises a mixture of wheat and barley plants, with a mixture of grain and stem samples. For each of those samples,

the total carbon content is provided along with the Mo content on a dry weight basis. However, in the data in the Excel files provided by SKB for this review, it is clear that one of those ten samples should have been rejected due to "*probable mineral contaminated sample"*.

With respect to the soil samples, 25 of the 28 samples were also reported in Sheppard et al. (2011), and correspond to soil samples collected at a depth of 0.2-0.25 m. A variety of soil types, both inorganic and organic is included: glacial clay, clayey gyttja, clayey till, cultivated peat and wetland peat. The remaining three samples, again a mixture of inorganic and organic soils, are taken from a depth of 0.3-0.35 m, with the data reported in Sheppard et al. (2009). A further four samples collected at the same depth and also reported in Sheppard et al. (2009) are also contained in the database, but have not been used, without any explanation.

The implications of these two factors on the calculated distribution of cR_agri_Cereal for Mo are shown in Table 22 below. When reporting to only two significant figures, if the original 28 soil samples are used then the mistake of not excluding one of the cereal samples when calculating the distribution for cR_agri_Cereal does not make any difference. Examination of this parameter in the Ecolego model file shows that the mistake was made as the value given is 1.23135478058668 kgdw kgC^{-1} (of the reporting of 15 significant figures suggest an uncritical approach to reporting of this parameter). Thus, it would appear that they have not ignored the data which have been incorrectly transferred into the database in Step 3 of the process outlined above, in this instance at least.

However, inclusion of those extra four soil samples leads to a wider distribution, with a lower geometric mean. The single value reported in IAEA (2010), when converted to kg dw kgC^{-1}, sits within these distributions[30].

Table 22: cR_agri_Cereal for Mo (kg dw kgC^{-1}) as used in SR-PSU and as rederived using the site data provided for this review. The rederived GM and GSD are show as both 4 significant figures. and 2 significant figures.

Origin	No. soil samples	No. cereal samples	GM	GSD	Min	Max
K_d and CR Report	28	10	1.2	3.2	7.2E-2	1.3E+1
Calculated for this review	28	10	1.231 (1.2)	3.182 (3.2)	7.2E-2	1.3E+1
	28	9	1.245 (1.2)	3.229 (3.2)	7.2E-2	1.3E+1
	32	10	1.018 (1.0)	3.518 (3.5)	2.7E-2	1.3E+1
	32	9	1.029 (1.0)	3.567 (3.6)	2.7E-2	1.3E+1
IAEA (2010)	1	1	1.818	-	-	-

Thus, if the more complete set of site data had been used then the deterministic dose associated with ingestion of Mo-93 contaminated cereals could have been reduced by up to 16.4%. The implications of using the more complete data set is shown in

[30] This is a single data point, reported as 8E-1 kg dw kg^{-1} dw, which has then been converted using a 0.44 kgC kg^{-1} dw as cited in Table F-1 of Tröjbom et al. (2013).

Figure 17; these are results from the deterministic model, with the only change being the cR_agri_Cereal value for Mo. Only two exposure groups are assumed to consume cereal: the drained mire farmer and the infield-outfield farmer.

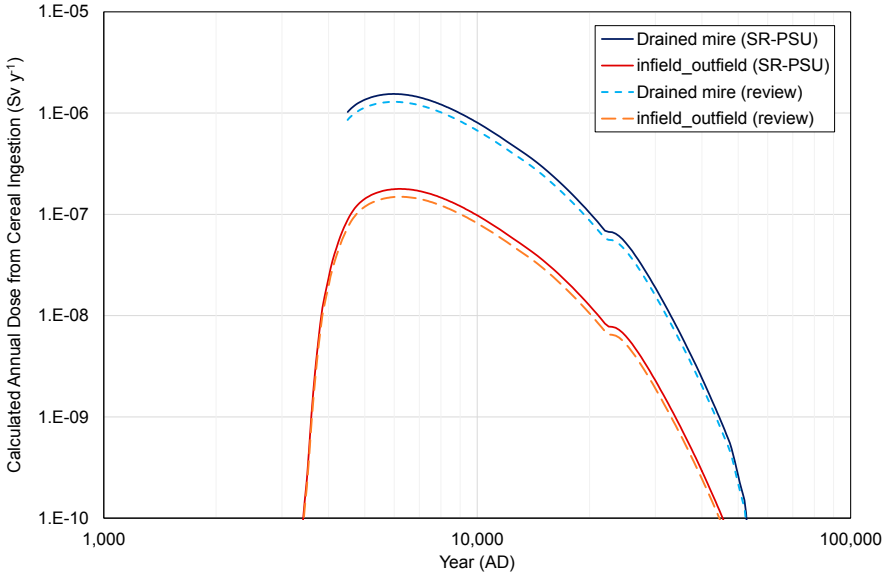

Figure 17: Effect of alternative cR_agri_Cereal values for Mo-93 on deterministic calculated annual doses from ingestion of cereal (Sv y^{-1}). The curves indicated as "SR-PSU" use the best estimate as reported in Table 6-19 of the Kd and CR Report, and the curves indicated as "review" use the geometric mean of 1.029 reported in Table 22 above.

4.5.2. Rederivation of Kd_regoPeat for Mo

Section 5.4 of the K_d and CR Report states that the available site data representing the RegoPeat compartment are "*wetland peat samples from 5 sites taken at a depth of 0.5 m*", and are reported in Sheppard et al. (2011). However, when calculating a Kd_regoPeat distribution for Mo, as with a small number of other elements, six rather than five paired site data are used (see Tables 5-8 and 5-9 in the K_d and CR Report). The identity of this extra data point was only made available via supplementary information that SKB supplied in response to queries from the initial phase review. This extra data point is that of a soil-pore water sample that was taken in Forsmark in an organic soil at a depth of 0.3-0.35 m, reported in Sheppard et al. (2009). There is no explanation given as to why this extra data point has been used for radionuclides where that sample had non-negative measurements in both the soil solid and pore water. Using the supplementary information and the SKB methodology, it is possible to verify the distribution used by SKB.

With regards to the Kd_regoPeat derived by SKB using the site data, the K_d and CR Report notes that the "*plausible*" interval obtained using site data for Mo (0.65-24 m^3 kg^{-1}) is significantly higher than the interval for literature data (0.007-0.13 m^3 kg^{-1}); see also the cumulative distribution functions for Kd_regoPeat in Figure 18. They suggest that this might be a site-specific property related to the chemical environment at Forsmark, and therefore use the site data in preference to the literature data.

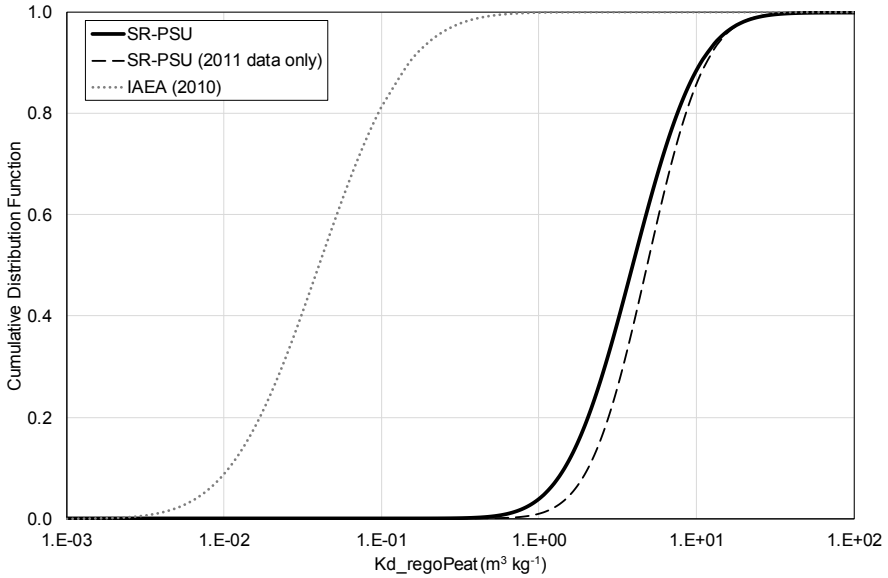

Figure 18: Cumulative distribution function of Kd_regoPeat for Mo. Figure shows the distribution used in SR-PSU, the distribution if only the five wetland samples from Sheppard (2011) were used, and also the distribution in IAEA (2010).

4.5.3. Consideration of Kd_regoPG for Molybdenum

Appendix F of the Radionuclide Transport Report notes Kd_regoPG as being one of the three key parameters in the sensitivity analysis with respect to the calculated human dose from Mo-93 exposure.

As is noted in Section 5.3 of the K_d and CR Report, the site data for molybdenum gives a higher K_d than that recommended in IAEA (2010) for all soils. Furthermore, the variation is larger than what SKB determined to be their GSDmax value for this parameter.

SKB state that there are no indications in the underlying site data that any of the values are less reliable. Furthermore, they suggest that the combination of data from marine and terrestrial sediments could perhaps contribute to the extended variation, for example due to redox effects. Certainly, the K_d for molybdenum calculated independently from the two paired marine sediment-pore water samples from Forsmark (~3.5 m^3 kg^{-1}) is greater than the range of values calculated for the seven paired terrestrial soil-pore water samples from both Forsmark and Simpevarp (0.039 to 0.84 m^3 kg^{-1}).

4.5.4. Non-Human Biota Exposure

As noted in Section 3.4 of the initial phase review (SSM, 2016), the documentation makes it clear that the non-human biota assessment is based on the ERICA assessment approach, and that the ERICA model and data has been implemented in Ecolego. Jaeschke et al. (2013)[31] describes the November 2012 version of ERICA as the starting point for that used in the SR-PSU assessment.

[31] Appendix A of Jaeschke et al. (2013).

Since the SR-PSU assessment was undertaken, a new version of ERICA, Version 1.2, was released in November 2014. The accompanying release note, ERICA (2014), notes that the new version of the software now includes a set of default parameter values for some radionuclides, such as Pa-231, that were not previously available, and that the Dose Conversion Coefficients for the external exposure of lichens and bryophytes were completely updated due to discrepancies in the original dataset.

In the initial review phase it was noted that key organisms in terms of exposure were (wading) birds, lichens and bryophytes in the marine, freshwater and terrestrial ecosystems. C-14 was the dominant radionuclide for the (wading) birds, and U-238 was the key radionuclide for lichen and bryophyte exposure. Consideration is given here with regards to the underlying assumptions supporting those particular non-human biota dose calculations.

Uptake of C-14 by (Wading) Birds

Section 10.2.2 of Biosphere Model Report states that the C-14 activity in any freshwater or marine biota is equal to the specific activity of C-14 of inorganic carbon in water in the solute phase, scaled by the fraction of carbon in the whole body of that organism.

While such an assumption may be valid for some organisms, birds do not spend 100% of their time in the water. According to Table 8-1 of the Radionuclide Transport Report, the times of the calculated peak doses to the marine and freshwater non-human biota occur at 4250 and 4500 y AD respectively. It should be noted that object 157_2 does not have a lake, and so for the freshwater exposure, the concentration of C-14 in dissolved form in the upper regolith is used for the dose calculations (see Section 10.2.2 of the Biosphere Model Report).

The question arises as to whether the assumption of birds spending 100% of their time in the water, with no time in the atmosphere, leads to a potential over-estimate of the exposure of the birds to C-14. If it is assumed that exposure in the atmosphere is external only, then spending 100% of its time in the atmosphere a (wading) bird would get a calculated dose of up to 5.9E-7 μGy h^{-1}, based on the atmospheric concentration at 4500 yAD, which is several orders of magnitude lower than the doses reported in Table 8-1 of the Radionuclide Transport Report.

Since the calculated maximum dose rates for (wading) birds are several orders of magnitude below the ERICA screening dose rate (10 μGy h^{-1}), the conservativism around the occupancy assumptions does not merit further consideration.

Table 23: Calculations of C-14 org in environmental media in biosphere object 157_2 for the main scenario[32]

Model input/output	4000 yAD	4250 yAD[33]	4275.7 yAD	4500 yAD
area_obj_aqu (m^2)	3.67E+4	3.5E+3	0	0
z_water (m)	8.3E-1	7.7E-2	0	0
Volume of water > 10 m^3 [34]	Yes	Yes	No	No
area_obj_ter (m^2)	1.32E+5	1.46E+5	1.47E+5	1.47E+5
C-14 org in environmental media in object 157_2				
AC_aqu_D (Bq m^{-3})	0	0	-	2.2E+1
AC_regoUp_ter_D (Bq m^{-3})	2.0E+1	2.1E+1	-	2.2E+1
Atmosphere_aqu (Bq)	1.7E+8	2.4E+8	-	2.4E+8
Atmosphere_ter (Bq)	1.6E+10	3.2E+10	-	4.9E+10
Derived C_atmos (Bq m^{-3}) [35] derived using 10 m atmosphere height	1.3E+2	6.8E+3	-	3.3E+4

Uptake of U-238 by Lichens and Bryophytes

With regards to non-human biota, in the terrestrial environment it is the lichen and bryophytes which are the most exposed organism type for the majority of the calculation cases considered (see Table 8-1 of the Radionuclide Transport Report). Further, the dominant radionuclide for the lichen and bryophyte exposure is U-238. Consideration is therefore given here as to the assumptions relating to the uptake of U-238 by these organisms.

As was noted above, one of the major changes in ERICA Version 1.2 is the values used for the Dose Conversion Coefficients for the external exposure of lichens and bryophytes. The value used in the SR-PSU assessment, as reported in Table E-6 of the Biosphere Parameter Report, is 4.6E-13 (μGy h^{-1})/(Bq kg^{-1} dw). However, the value in ERICA Version 1.2 is 5.0E-8 (μGy h^{-1})/(Bq kg^{-1} dw), some five orders of magnitude greater. Despite this large discrepancy, the external dose to lichens and bryophytes makes an insignificant contribution to the total dose from U-238 exposure, which is dominated by internal dose.

In the remainder of this section, focus is therefore given to the two factors which will affect the calculated internal dose to lichens and bryophytes following U-238

[32] Area_obj_aqu is the area of water in a given biosphere object; z_water is the mean depth of the water body'; area_obj_ter is the area of land in a given biosphere object; AC_aqu_D is the volumetric concentration of dissolved radionuclide in the water; AC_regoUp_ter_D is the volumetric concentration of dissolved radionuclide in the top soil layer in the mire; Atmosphere_aqu is the inventory of a radionuclide in the atmosphere above a water body in a given biosphere object; Atmosphere_ter is the inventory of a radionuclide in the atmosphere above land in a given biosphere object; and C_atmos is the volumetric concentration of C-14 in the atmosphere.
[33] Areas calculated based on the values given at 4000 y AD and 4275.7 y AD in Table C-5 of the Biosphere Parameter Report.
[34] In the Ecolego code, 10 m^3 is the minimum volume set to have a water body in biosphere object 157_2.
[35] These values are derived using a total atmosphere height of 10 m (see Section 8.9 and 9.5.3 of the Biosphere Parameter Report), and if water is present area_obj_aqu to estimate the volume of air present. In the absence of water, then area_obj_ter is used instead.

exposure. These are the concentration ratio for lichens and bryophytes (cR_Ter_pp_lichen_NHB), and the internal Dose Conversion Coefficient.

Using the supplementary information provided by SKB for this stage of the review, it is possible to extract all the data points from their database required to calculate cR_Ter_pp_lichen_NHB for U. In particular, only soil samples where *aqua regia* digestion was used prior to the sample analysis were considered by SKB. This is claimed to then maximise the CR's derived from the site data[36]. Using this restriction on the soil samples, there are 28 soil solid and three bottom layer samples from Forsmark with non-negative activities of U reported. There are eight soil solid and four bottom layer samples from Simpevarp with non-negative activities of U reported. These activities are all reported in mg kg^{-1} dw. Note that the CR used for non-human biota are reported in kg dw kg^{-1} fw, meaning that the concentrations of U in the bottom layer samples need to be multiplied by their dry matter content to obtain a concentration in mg kg^{-1} fw prior to deriving the CRs. Following SKB's methodology, as site specific dry matter content data was available for all of these samples (range of 25.7 % to 88.9 %), those values should have been used here to convert the concentrations of U in the bottom layer samples rather than the generic value in IAEA (2010), 24 % (see also Table F-1 of the K_d and CR Report). However, in trying to recreate the distribution reported by SKB in the K_d and CR Report, the GSD's reported in Table 6-2 can only be almost reproduced if the IAEA (2010) conversion factor is used.

The independently calculated GSD's using the Forsmark data are lower than those reported by SKB (Table 24); note that the minimum and maximum of the distributions from the SR-PSU assessment are the limits in calculated values, not the 5^{th} and 95^{th} percentiles of an assumed log-normal distribution.

Table 24: Distributions of cR-Ter_pp_lich_NHB (kg dw kg^{-1} fw) for U

Source	BE	GM	GSD	Min	Max	N
SR-PSU – from Table 6-3 of the K_d and CR Report	2.9E-2	2.5E-2	8.9	2.3E-4	7.6E+0	7
SR-PSU – verification	2.9E-2	2.5E-2	8.8	2.3E-4	7.6E+0	7
IAEA (2014)	-	1.3E0	3.2	2.0E-2	2.9E+1	237
ERICA Version 1.2	9.1E-1	-	-	-	-	-

The K_d and CR Report notes that the distribution for cR_Ter_pp_lich_NHB is wide due to variations in U concentration in the soil samples. In the Forsmark data, one of the bottom layer concentrations of U is greater than the concentration of U in 10 of the soil samples. It is therefore not possible to ascribe the width of the distribution to the ranges of either the soil or the bottom layer activities of U.

The second factor to consider is the assumed internal Dose Conversion Coefficients (Table 25). It is noticeable that some of the zero values assumed in the SR-PSU assessment have been assigned non-zero values in ERICA Version 1.2.

[36] p34 of the K_d and CR Report.

Table 25: Internal Dose Conversion Coefficients for U-238 (μGy h^{-1})/(Bq kg^{-1} dw)

Source	DCC_int_alpha	DC_int_beta_gamma	DCC_int_low_beta
SR-PSU [37]	2.4E-3	0	0
ERICA Version 1.2	2.41E-3	5.21E-6	6.68E-7

As part of this review, consideration is given to the potential implications of the differences in the exposure calculations highlighted above on the total dose to lichens and bryophytes from U-238 exposure. The peak calculated concentration of U-238 in the soil in the reference case[38] is 3.17 Bq kg^{-1} dw, occurring at 7050 AD. Using ERICA Version 1.2, the calculated total dose to lichen and bryophytes is 6.96E-2 μGy h^{-1}. Whilst this is more than a factor of 20 greater than the total dose reported in SKB (2014b), 3.3E-3 μGy h^{-1}, it is still several orders of magnitude below the 10 μGy h^{-1} screening level for potential impacts to non-human biota.

4.6. Conclusions of K_d and CR Review

The main conclusions from in-depth review of the derivation of K_d and CR values for the SR-PSU assessment are summarised below.

- The highly automated process(es) of extracting site-specific data from SKB's data archives, and using these to calculate and 'quality assure' K_d and CR values, is complex but ultimately traceable with the aid of the additional explanatory documents provided by SKB.
- This traceability is less obvious when reading the original K_d and CR Report.
- Even given the explanation of the automated data handling processes, the complexity of these procedures may lead to a loss of focus on the importance of the parameter values produced. The eventual statistical power of the site-specific parameters obtained is limited by low numbers of data pairs from which K_ds and CRs can ultimately be calculated (e.g. N=7 for lower regolith K_d for nickel; N=1 for CR for nickel in fish).
- Several methods have been applied to compensate for this lack of statistical power, including the use of the statistical variation of ALL elements to represent plausible variation in a parameter for a single element. This approach is arbitrary and may reflect a pragmatic need to increase the apparent statistical power of the data analysis in the face of very low numbers of site-specific parameter values available to SKB.
- SKB concedes that the process of defining the plausible limits of CRs and K_ds is "*to some extent subjective and based on the general assumption that it is conservative to widen the PDFs of selected parameter data*" based on the use of GSDs for all elements.
- A more richly-replicated site-specific database (i.e. more and better-targeted measurements at Forsmark and Laxemar-Simpevarp) would have circumvented the need for such complex and debatable statistical approaches. It would also have reduced the reliance on, and influence of, the authoritative but ultimately limited literature sources incorporated within the SR-PSU assessment.

[37] Data from Tables E-8, E-13 and E-14 of the Biosphere Parameter Report.
[38] As determined using LandscapeMainChain_CC1.eas, running in deterministic mode.

As part of the review process, SKB's methodology was followed to derive two of the parameters identified by SKB as being important in explaining variations in the dose in probabilistic calculations with regards Mo-93 exposure (see Section 4.5).

In using site data to determine the value of the concentration ratio to cereal crops, it has been found that an inconsistent usage of their own methodology means that SKB may have overestimated the potential exposure from the ingestion of Mo-93 contaminated cereal. However, using the value recommended in IAEA (2010) would lead to a further increase in the calculated dose.

For all K_ds except those for the lower regolith and glacial clay, the values obtained by SKB using their site-specific data for molybdenum are either greater than, or towards the upper end of the values reported in the literature (e.g. IAEA, 2010). This is particularly true of the K_d for post-glacial deposits, for which a combination of terrestrial soil and marine sediment data were used to derive the K_d distribution. The use of the site-specific parameterisation for K_d therefore leads to more molybdenum being retained in the upper soil layers, which are those that are more likely to interact directly with plants, and thus higher calculated doses. It should be noted that the number of site specific samples (5-10) is approximately the same as that used in IAEA (2010), nine samples.

Given the dominance of molybdenum in the calculation of total doses in the assessment, there is merit in undertaking a further literature review to ascertain if any further data have become available since IAEA (2010) was published. It would also be worthwhile re-examining the sample selection procedure used by SKB in determining which samples were used in defining the distribution of each K_d.

5. Conclusions

The SR-PSU assessment adopts a complicated approach to representing potential contamination of the biosphere and its radiological significance over the time scale of tens of thousands of years. SR-PSU represents a further iteration on previous assessments for the SFR facility. Iteration and the proximity of some of the calculated results to the risk criteria in previous assessments for SFR provide drivers for some of the complexity in the modelling approach, along with interpretation of the significant amount of information derived from characterisation of the present-day biosphere.

The significant uncertainties inherent in projecting potential consequences of radioactive waste disposal over extremely long periods mean that assessment results can only be taken as broad indicators of environmental safety and are typically based on conservative assumptions with regards to potential exposure. The degree of complexity in the biosphere modelling approach, together with a combination of assumptions with regards to radionuclide releases to the biosphere and potential exposures, mean that some conservatisms have been removed in relation to previous assessments.

The principal conclusions from the main review phase for the SR-PSU assessment with regards to biosphere modelling for specific radionuclides are summarised below. These findings are drawn from three review activities, which were prioritised based on the initial review phase:

- independent implementation of the SR-PSU biosphere models with a view to verifying results and gaining a thorough understanding of the modelling approach adopted;
- in-depth review of the modelling of C-14; and
- detailed review of the derivation of parameter distributions for K_d and CR.

The findings should be read in conjunction with those of the initial review phase.

The main conclusions drawn from independently implementing the SR-PSU biosphere model in AMBER are summarised below.

- The biosphere mode is extremely complicated, requiring 280 equations in the Biosphere Model Report, and 56 compartments/158 transfers in a cut-down implementation. Nonetheless, the model and data are comprehensively documented and have permitted the results to be largely reproduced (to within about a factor of two).
- The modelling approach represents a hybrid between a probabilistic and deterministic model, in which PDFs are assigned to a very large number of biosphere parameters while key aspects of the modelling are represented deterministically. The distribution of results from probabilistic calculations is therefore an incomplete measure of parameter uncertainty.
- The Ecolego modelling makes use of deterministic ‘hard-wired’ values for some key parameters, including peat thickness and scaling factors used for agricultural soil concentrations, in a way that makes the values used inconsistent with underlying parameters in probabilistic calculations.
- Simplifying assumptions exacerbate the rapid rate of loss of C-14 to the atmosphere, notably the neglecting of horizontal water flows in sub-surface layers in the terrestrial modelling.
- The Ecolego implementation was found to differ from the model specification in calculating radionuclide concentrations in drained mire

soils in a way that underestimates the results by about a factor of five (i.e., if SKB's model specification is correct, then the SR-PSU results for the drained mire farmer should be about a factor of five higher).

- Human habit assumptions result in a relatively low degree of exposure for some of the exposure groups, notably:
  - very low capture fractions for drilled wells;
  - the drained mire and garden plot groups spend only 54 hours per year on contaminated soils;
  - the garden plot group obtains only 8% of their dietary carbon from the goods that they produce;
  - the larger hunter-gatherer group is the only one that consumes fish, which was a key exposure pathway in previous assessments;
  - the equivalent of 30 adult individuals being used as a basis for the hunter-gatherer group effectively dilutes exposure in comparison to other groups such that only 0.7% of dietary intake comes from the most contaminated biosphere object after terrestrialisation.
- Explicit dynamic modelling of agricultural soil concentrations reproduced the results of the analytical approach adopted in SR-PSU for drained mire soils with the exception of relatively short-lived radionuclides, for which the analytical approach was found to underestimate concentrations.

The main conclusions drawn from review of the SR-PSU biosphere model for C-14 are summarised below.

Conclusions regarding the regolith:

- Organic carbon pools have been explicitly introduced to improve the way that the carbon balance is represented.
- The existence and distinction in the behaviour of $^{14}CH_4$ in regolith layers, notably in the mire, is not discussed at all and is completely neglected in the biosphere modelling.

Conclusions regarding the aquatic ecosystem:

- The assumed release to biosphere object 157_2, which does not have a water body, means that people are less exposed to contaminated fish (much of the C-14 degasses from the mire surface before reaching the lake that is present in Object 157-1), the consumption of which dominated the C-14 dose in the SAR-08 assessment.
- The modelling approach adopted for C-14 accumulation in fish results in significantly lower concentration ratios when compared against IAEA recommended values.

Conclusions regarding the terrestrial ecosystem:

- The assumed degassing rates from soil are much higher than those used in other assessments. There is potential for further comparison of the rates against more recent literature sources.
- The assumed refractory organic matter content is lower than might be expected for mire vegetation such as *Spaghnum* moss. This leads to a greater proportion of decayed matter entering the soil pore water, for release to the atmosphere, than might be appropriate for such ecosystems

Conclusions regarding the atmospheric sub-model:

- The new atmospheric exchange model provides an improved representation of micrometeorological processes. Similar models have been adopted by other waste management organisations in support of their safety assessments over recent years.

The main conclusions from an in-depth review of the derivation of K_d and CR values for the SR-PSU assessment are summarised below.

- The automated process(es) of extracting site-specific data from SKB's data archives, and using these to calculate and 'quality assure' K_d and CR values, is highly complex but ultimately traceable with the aid of the additional explanatory documents provided by SKB.
- This traceability is less obvious when reading the original K_d and CR Report.
- Even given the explanation of the automated data handling processes, the complexity of these procedures may lead to a loss of focus on the importance of the parameter values produced. The eventual statistical power of the site-specific parameters obtained is limited by low numbers of data pairs from which K_ds and CRs can ultimately be calculated (e.g. N=7 for lower regolith K_d for nickel; N=1 for CR for nickel in fish).
- Several methods have been applied to compensate for this lack of statistical power, including the use of the statistical variation of ALL elements to represent plausible variation in a parameter for a single element. This approach is arbitrary and may reflect a pragmatic need to increase the apparent statistical power of the data analysis in the face of very low numbers of site-specific parameter values available to SKB.
- SKB concedes that the process of defining the plausible limits of CRs and K_ds is "*to some extent subjective and based on the general assumption that it is conservative to widen the PDFs of selected parameter data*" based on the use of GSDs for all elements.
- A more richly-replicated site-specific database (i.e. more and better-targeted measurements at Forsmark and Laxemar-Simpevarp) would have circumvented the need for such complex and debatable statistical approaches. It would also have reduced the reliance on and influence of the authoritative but ultimately limited literature sources incorporated within the SR-PSU assessment.

As part of the review process, SKB's methodology was followed to derive two of the parameters identified by SKB as being important in explaining variations in the dose in probabilistic calculations with regards Mo-93 exposure (see Section 4.5). Given the dominance of Mo-93 to the total calculated doses in the assessment, there is merit in undertaking a further literature review to ascertain if any further molybdenum K_d data has become available since IAEA (2010) was published. It would also be worthwhile re-examining the sample selection procedure used by SKB in determining which samples were used in defining the distribution of each K_d.

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Review of analysis of dose to non-human biota in SR-PSU (in Swedish with English abstract)

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Registration number: SSM2016-250
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Abstract

The Swedish Nuclear Fuel and Waste Management Co. (SKB) has applied to extend the SFR facility for low- and intermediate-level radioactive waste. This report is part of SSM's review of SKB's long-term safety analysis called SR-PSU. The safety analyses concerns the safety after closure of SFR and is part of the licence application. The aim of this assignment was to review the risk assessment for non-human biota. The review was conducted from the viewpoint of current laws and regulations. In total six SKB reports were reviewed in which focus was on relevant parts for the risk assessment for non-human biota. The results of this review show that SKB, in general, uses an internationally accepted method, the ERICA-tool (transferred to Ecolego) in the screening dose calculations to non-human biota. The calculations result in dose rates below internationally recommended screening dose rates for protection of the environment. However, SKB will have to clarify and explain some assumptions made in the risk assessment that lack an environmental perspective. In total, nine questions were identified during this review that would need further clarification or explanation. SKB's assumptions regarding biosphere object size that effects the radionuclide concentrations in ecosystems and SKB's assumptions about radionuclide uptake in non-human biota can be mentioned as examples of such questions. In conclusion, further clarification is needed from SKB to facilitate an evaluation of the conservatism in SKB's risk assessment for non-human biota.

Sammanfattning

Svensk Kärnbränslehantering AB (SKB) har ansökt om att bygga ut SFR, slutförvaret för kortlivat låg- och medelaktivt radioaktivt avfall. Denna rapport är en del av SSM:s granskning av SKB:s långsiktiga säkerhetsanalys SR-PSU. Säkerhetsanalysen gäller säkerheten efter förslutning av ett utbyggt SFR och ingår i SKB:s licensansökan för utbyggnad av SFR. Syftet med denna granskning har varit att granska utvärderingen av radiologiska effekter på andra organismer än människor. Granskning har utförts med utgångspunkt i gällande lagar och föreskrifter. Totalt har 6 SKB rapporter ingått i granskningen där relevanta delar för utvärderingen av radiologiska effekter på andra organismer än människa granskats. Resultaten visar att SKB generellt använder en internationellt accepterad metod, ERICA-verktyget (överfört till Ecolego), för att beräkna screening dosrater till biota. Beräkningarna resulterar i dosrater som ligger under internationellt rekommenderade screening dosnivåer för biota inom strålskyddet av miljön. Dock kan det konstateras att SKB behöver förtydliga och motivera varför vissa antaganden i utvärderingen inte har ett miljöperspektiv. Totalt har nio punkter och frågor identifierats under granskningen som skulle behöva förtydligas eller kompletteras. Som exempel kan nämnas SKB:s antaganden om biosfärsobjektens storlek som påverkar radionuklidkoncentrationerna i ekosystem media och antaganden om upptag av radionuklider i biota i olika ekosystem. Förtydliganden behövs för att möjliggöra en bedömning om SKB:s utvärdering av radiologiska effekter på andra organismer än människa är konservativ.

Innehåll

1. Granskning av dosrater till andra organismer än människor

Denna rapport är en del av SSM:s granskning av SKB:s långsiktiga säkerhetsanalys SR-PSU. Säkerhetsanalysen gäller säkerheten efter förslutning av SFR och ingår i SKB:s licensansökan för utbyggnad av slutförvaret för kortlivat låg- och medelaktivt avfall. Granskningen har utförts av Karolina Stark under två månader vid Institutionen för ekologi, miljö och botanik, Stockholms universitet, enligt kontrakt SSM 2016-250-1 mellan Stockholms universitet och SSM. Denna rapport innehåller Karolina Starks sammanfattning av resultaten av granskningen och uppkomna frågor där förtydligande eller kompletterande information kan behövas från SKB.

1.1. Syftet med denna granskning

Syftet med denna del av granskningen har varit att granska utvärderingen av radiologiska effekter på andra organismer än människor, speciellt om den presenterade utvärderingsmetoden tar hänsyn till alla relevanta transport- och ackumulationsprocesser, radionuklider och organismer. Det har även ingått att granska om de parametervärden som använts för dosmodellering vad gäller andra organismer än människor är relevanta för den tänkta platsen och om de överensstämmer med de parametervärden som använts i SR-PSU vid modellering av doser till människa. Slutligen ingick även att granska om de dos-effekt samband som använts är relevanta för att utvärdera sannolikheten för radiologiska effekter på andra organismer än människa.

1.2. Aktuella lagar och föreskrifter

Denna granskning av utvärderingen av radiologiska effekter på andra organismer än människa i SKB:s långsiktiga säkerhetsanalys har utförts med utgångspunkt i gällande lagar och föreskrifter; Miljöbalken 1998:808, Strålskyddslagen 1988:220 och SSM:s föreskrift SSMFS 2008:37. I SSMFS 2008:37 paragraf 6 och 7 och i de allmänna råden med bilaga 2 står följande:

- **6 §** ”Slutligt omhändertagande av använt kärnbränsle och kärnavfall ska genomföras så att biologisk mångfald och hållbart nyttjande av biologiska resurser skyddas mot skadlig verkan av joniserande strålning.”

- **7 §** **”**Biologiska effekter av joniserande strålning i berörda livsmiljöer och ekosystem ska redovisas. Redovisningen ska bygga på tillgänglig kunskap om berörda ekosystem och ta särskild hänsyn till förekomst av genetiskt särpräglade populationer, såsom isolerade populationer, endemiska arter och utrotningshotade arter samt i övrigt skyddsvärda organismer.”

  Biosfärsförhållanden och exponeringsvägar
  ”De framtida biosfärsförhållandena för beräkningar av omgivningskonsekvenser för människa och miljö bör väljas så att de är överensstämmande med det klimattillstånd som antas råda. Om det inte är uppenbart orimligt bör dock dagens biosfärsförhållanden vid slutförvaret och dess omgivningar utvärderas, d.v.s. jordbruksmark, skog, våtmark (myr), insjö, hav eller andra relevanta ekosystem. Vidare bör hänsyn tas till landhöjning (-sänkning) och andra förutsägbara förändringar.

Riskanalysen kan innehålla ett begränsat urval av exponeringsvägar, men valet av dessa bör baseras på en analys av den mångfald av mänskligt utnyttjande av miljö- och naturresurser som kan förekomma i Sverige idag. Hänsyn bör även tas till att enskilda individer kan beröras av kombinationer av exponeringsvägar inom och mellan olika ekosystem."

Miljöskydd
"Beskrivning av exponeringsvägar enligt ovan bör utföras så att de också inkluderar exponeringsvägar till vissa organismer i de ekosystem som angivits ovan och som bör ingå i riskanalysen. Koncentrationen av radioaktiva ämnen i jord, sediment och vatten bör redovisas där så är relevant för respektive ekosystem.

När biologisk effekt för de identifierade organismerna kan förmodas, bör en värdering göras av vilken konsekvens detta kan ha för de berörda ekosystemen, med syfte att möjliggöra bedömning av betydelse för biologisk mångfald och ett hållbart nyttjande av miljön.

Den analys av konsekvenser för organismer i "dagens biosfär" som genomförs enligt ovan bör användas för bedömningen av miljömässiga konsekvenser i ett långtidsperspektiv. För antagna klimat där dagens biosfärsförhållanden är uppenbart orimliga, t.ex. ett kallare klimat med permafrost, är det tillräckligt att göra en översiktlig analys baserad på idag tillgängliga kunskaper om tillämpliga ekosystem."

Råd om utvärdering av miljöskydd
"De organismer som tas med i analysen av miljöpåverkan bör väljas utifrån deras betydelse i ekosystemen, men också utgående från deras skyddsvärde enligt övriga biologiska, ekonomiska eller naturvårdsmässiga kriterier. Med övriga biologiska kriterier avses bland annat genetisk särprägling och isolation (t.ex. i dag kända endemiska arter), med ekonomiska kriterier avses organismernas betydelse för olika slag av näringsfång (t.ex. jakt och fiske), och med naturvårdsmässiga kriterier om de omfattas av skydd enligt gällande lagstiftning eller lokalt utformade regler. Övriga aspekter, t.ex. kulturhistoriska, bör också beaktas i identifieringen av sådana organismer.

Bedömning av effekter av joniserande strålning i valda organismer, härrörande från radioaktiva ämnen som kan ha spridits från ett slutförvar, kan göras utifrån den generella vägledning som ges i den Internationella strålskyddskommissionens (ICRP) Publikation 91.[1] Tillämpligheten av de kunskaper och databaser som används avseende spridning av radioaktiva ämnen i ekosystem och strålningens effekter på olika organismer bör bedömas och redovisas.

[1] A Framework for Assessing the Impact of Ionising Radiation on Non-human Species, ICRP Publication 91, Annals of the ICRP 33:3; 2003"

2. Granskningsresultat från utvärderingen av radiologiska effekter på andra organismer än människor

I detta kapitel sammanfattar jag vilka metoder, processer, radionuklider, organismer, parametervärden och dos-effekt samband som jag har uppfattat att SKB använt för att utvärdera radiologiska effekter på andra organismer än människa i SR-PSU.

2.1. SKB:s metoder och dosrat-resultat

I sin långsiktiga säkerhetsanalys SR-PSU enligt TR-14-01 använder SKB dosverktyget ERICA:s tillvägagångsätt (Brown et al., 2008) för beräkning av exponering och absorberade dosrater till andra organismer än människa. ERICA är ett fritt tillgängligt dosverktyg avsett för screeningberäkningar av dosrater till organismer och används internationellt. SKB har beskrivit att dosverktyget ERICA beräknar absorberade dosrater från både extern strålning från radionuklider i jord, sediment och vatten och från intern strålning från upptagna radionuklider i organismens kropp. Organismens storlek (oftast en ellips), placering och uppehållstid, i tillgängliga ekosystem scenarion, ingår tillsammans med sönderfallsegenskaper för olika typer av radionuklider i beräkningar av dosomvandlingskoefficienter (DCC). Dessa dosomvandlingskoefficienter används sedan för att omvandla aktivitetskoncentrationer i media eller i organismen till absorberad dosrat för varje radionuklid. Alla interna och externa dosrater för samtliga radionuklider summeras till slut för varje organism till en total dosrat.

För dosberäkningarna i SR-PSU har dosverktyget ERICA överförts till Ecolego där beräkningarna utförts enligt R-13-46. Dosomvandlingskoefficienter från ERICA verktyget överfördes till biosfärsmodellen tillsammans med något modifierade uppehållstidsfaktorer (occupancy factor) för organismer i de tre tillgängliga ekosystemen marint, sötvattens- och terrest ekosystem (eller som SKB kallar dem: hav, sjö/å och våtmark) och ERICA:s viktfaktorer för olika typer av strålning. Därefter beräknade SKB dosrater till organismerna för varje biosfärsobjekt genom användandet av lokala aktivitetskoncentrationer där sådana fanns tillgängliga i aktuellt medium. I akvatiska ekosystem beräknades internexponering baserat på aktivitetskoncentrationer av radionuklider lösta i vatten medan den externa exponeringen beräknades från den totala aktiviteten från både lösta och partikulärt bundna radionuklider. Detta är en modifikation av ERICA verktyget som rekommenderar att aktivitetskoncentrationer från filtrerat vatten ska användas för extern exponering. Aktivitetskoncentrationer i akvatiska ytsediment användes för att beräkna extern exponering till organismer som lever i eller på sedimenten. I terrestra ekosystem beräknades intern och extern exponering från aktivitetskoncentrationer i våtmarkstorv.

Biosfärsobjektet 157_2 har inget identifierat sjö-stadium då SKB modellerat att det kommer att utvecklas från en havsvik till en våtmark. Dock är det troligt att grunda dammar kommer att förekomma i objektet under landfasen varför aktivitetskoncentrationer i porvatten från våtmarken använts för att beräkna dosrater till sötvattensorganismer i detta objekt. Extern exponering till sötvattensorganismer från sediment beräknades baserat på aktivitetskoncentrationer i våtmarkstorv.

SKB beräknade dosrater till biota för flera olika modelleringsfall och scenarion där huvudfallet kallas *global warming variant*. De högsta doserna återfanns alltid där

radionuklider från förvaret når biosfären direkt från geosfären och det var i objekt 157_2. Därför har SKB fokuserat på att göra exponeringsberäkningar för biota i just detta objekt med ett undantag för beräkningar i ett *early periglacial climate variant*-scenario och beräkningar nedströms objekt 157_1 där radionukliderna transporteras med ytvatten. Ett antal beräkningar har även gjorts för mindre sannolika scenarion och kombinationer av olika scenarion.

I huvudscenariot *global warming variant* i det marina ekosystemet var de beräknade högsta dosraterna enligt TR-14-01 tre storleksordningar lägre än screening-värdet 10 μGy h^{-1}. Den högsta dosraten beräknades till vadande fågel på 5,2 x 10^{-3} μGy h^{-1} främst från ^{14}C. I sötvattensekosystem beräknades de högsta dosraterna till fågel på 7,1 x 10^{-3} μGy h^{-1} främst från ^{14}C och till zooplankton i samma dosratnivå. I terrestra ekosystem beräknades de högsta dosraterna till lavar och mossor på 3,3 x 10^{-3} μGy h^{-1} främst från ^{238}U och även till detritivorer i samma storleksordning.

I andra SKB scenarion var de högsta beräknade dosraterna till fågel på 9,2 x 10^{-2} μGy h^{-1} i sötvattensekosystem i ett jordbävningsscenario och till bl a kärlväxter, zooplankton samt lavar och mossor i samma storleksordning för sju andra scenarion (Se Tabell 9-22 i TR-14-01).

2.2. Transport- och ackumuleringsprocesser

SKB har i SR-PSU beräknat dosrater för många olika tänkbara scenarion där man tar hänsyn till olika processer (Se t ex TR-14-09). Utsläppen av och koncentrationerna av olika radionuklider beräknar SKB till olika biosfärsobjekt i landskapsmodellen. De resulterande radionuklidkoncentrationerna är dock beroende av biosfärsobjektets storlek vilket är den avgörande faktorn för hur mycket radionukliderna kommer att spädas ut efter ett utsläpp i modellen. Utgångspunkten för hur stora biosfärsobjekten kan vara är avrinningsområden och hur många människor som kan livnära sig i de olika objekten. Beräkningar för mindre storlek på objekten har gjorts i TR-14-06 men också här med människan som utgångspunkt. Resultaten av dessa beräkningar var att i det minsta objektet blev radionuklidkoncentrationerna en storleksordning större. Inga beräkningar av olika objektsstorlekar har gjorts baserat på vad andra organismer skulle behöva för yta för att överleva, enligt t. ex. deras hemområdesstorlek.

Enligt R-13-46 och R-14-02 har SKB gjort en analys av möjliga exponeringsvägar för människa vilka även antogs som relevanta för de flesta andra organismer. Dessa exponeringsvägar var exponering via inhalation, intag av föda, externstrålning, via huden och via direkt upptag i kroppen. SKB gör sedan inga specifika beräkningar för dessa olika exponeringsvägar för biota utan antar att de täcker in det mesta genom att använda ERICA-verktygets koncentrationskvoter (CR) för jord, sediment och vatten för de identifierade organismerna.

2.3. Radionuklider

Enligt en jämförelse av Tabell 10-1 och Tabell 10-2 i SKB rapporten TR-14-06 och enligt TR-14-01 så använder SKB samma radionuklider för beräkning av dosrater till andra organismer som används till beräkning av dos till människa. Dock har SKB uppdaterat inventariet av radionuklider för dosberäkningarna till människa i SR-PSU men detta har inte gjorts för andra organismer eftersom SKB ansåg att dosraterna ändå låg så pass långt under screeningvärdet på 10 μGy h^{-1}.

2.4. Organismer

Enligt R-14-02 och TR-13-23 har ett antal representativa arter identifierats av SKB baserat på tre kriterier utifrån SSMFS 2008:37. Dessa tre kriterier är:

- Organismer som är viktiga för det relevanta ekosystemet
- Hotade, endemiska eller genetiskt viktiga arter
- Arter av kommersiellt eller kulturellt värde (inte inkluderande tamdjur/boskap)

SKB har sedan jämfört sina representativa arter med ERICA verktygets referens organismer. SKB fann att ERICA:s referens organismer täckte in de platsspecifika arterna väl men lade även till egna så som mikrofytobentos, utter, roskarl och svarttärna. Totalt har SKB beräknat doser till 41 organismer (Tabell 1; 13 för sötvatten, 11 för marina, 14 för terrestra, 2 för marint och terrest däggdjur och fågel, och 1 för sötvattens och terrest fågel).

Tabell 1. Utvalda organismer som SKB beräknat dosrater till i SR-PSU: Översatt från TR-14-06 Tabell 7-3.

Terrest ekosystem	Marint ekosystem	Sötvattens-ekosystem	Marint och terrest eko.	Sötvatten och terrest eko.
Lavar och mossor	Växtplankton	Växtplankton	Utter	Svarttärna
Gräs och örter	Makroalger	Mikrofytobentos	Roskarl	
Buskar	Kärlväxter	Kärlväxter		
Träd	Djurplankton	Djurplankton		
Jordlevande evertebrater	Havsborstmask	Insektslarv		
Detritivorer	Bottenlevande mollusk	Musslor		
Flygande insekt	Kräftdjur	Gastropod		
Gastropod	Bottenlevande fisk	Kräftdjur		
Groddjur	Pelagisk fisk	Bottenlevande fisk		
Kräldjur	Vadande fågel	Pelagisk fisk		
Fågel	Däggdjur	Groddjur		
Fågelägg		Fågel		
Däggdjur (litet)		Däggdjur		
Däggdjur (stort)				

2.5. Parametervärden

Enligt TR-13-23 har SKB i SR-PSU på grund av att koncentrationskvoter (CR) har en stor inverkan på dosberäkningarna till biota använt sig av platsspecifika CR när dessa har varit tillgängliga. Där inga platsspecifika CR funnits så har man använt data från

ERICA-verktyget, använt andra radionuklider som analoger eller använt ICRP:s CR-värden. Enligt TR-13-23 antas organismerna inta föda från de ekosystem som de antas vistas i mest dvs SKB använder CR-värden för dessa ekosystem.

2.6. Dos-effekt samband

Då det inte finns något dosgränsvärde för biota i SSM:s föreskrifter så har SKB enligt TR-14-01 tittat på vad som rekommenderas internationellt. Generellt rekommenderas att använda ett screeningvärde där en dosrat under detta värde har låg sannolikhet att resultera i skadliga effekter på biota. Om dosraten skulle vara högre än screening-värdet så rekommenderas att man gör ytterligare och noggrannare dosberäkningar då det finns risk för effekter. SKB använder sig av screeningvärdet 10 μGy h^{-1} som också används i ERICA-verktyget. Eftersom ICRP har tagit fram dosratnivåer kallade DCRL (derived consideration reference level) för referens organismer (ICRP, 2008) som i vissa fall är lägre (ner till 4 μGy h^{-1}) än screeningvärdet i ERICA så jämför SKB även de beräknade dosraterna med de lägsta DCRL-nivåerna från ICRP.

Samtliga av SKB redovisade beräknade dosrater till biota är under både ICRP:s DCRL och ERICA-verktygets screeningvärde (Se Tabell 9-22 i TR-14-01).

3. Granskningsfrågor

3.1. Förslag till kompletterande information

I detta avsnitt redovisas de punkter och frågor som uppkommit under granskningen och för vilka jag har gjort bedömningen att SKB behöver förtydliga sitt resonemang kring utvärderingen av radiologiska effekter på andra organismer än människa och där förtydligande eller kompletterande information kan behövas från SKB.

1. I SR-PSU använder sig SKB av dosverktyget ERICA (överfört till Ecolego) i sina dosratsberäkningar till andra organismer än människa. Vilken version av ERICA har SKB använt?
2. En ny version av ERICA-verktyget släpptes i november 2014 i vilken ett antal uppdateringar hade gjorts så som uppdatering av CR-värden från databasen Wildlife transfer database, uppdatering av extrapoleringsmetoder när data saknas och ändring av placering och gruppering av några referens organismer samt borttagande av ”Fågelägg” som referens organism. Påverkar dessa uppdateringar av ERICA SKB:s beräkningar av dosrater och i så fall hur?
3. I TR-13-23 rekommenderas det att organismerna ska antas vara nära på/i jord och sediment i så stor utsträckning som möjligt i dosrat-beräkningarna då detta antagande är konservativt. Varför antas inte då groddjur befinna sig i jord (som nu är default i ERICA-verktyget) i terrestra ekosystem och i/på sediment i sötvattensekosystem? Och varför antas inte utter ha någon kontakt med sediment i marina ekosystem?
4. I geometrin för växter tar ERICA-verktyget inte hänsyn till rötter som befinner sig i jorden/sediment. Enligt TR-13-23 kan dosraten till dessa organismer därför vara underskattad. Hur motiverar SKB att de ändå använder geometrin för växter från ERICA? Hur mycket underskattas då dosraten?

5. Enligt Strålskyddslagen (SFS 1988:220) ska människor, djur och miljö skyddas mot skadlig verkan av strålning. Systemet för skydd av djur och miljö har utvecklats mycket och etablerat sig mer och mer under de senaste 10 åren. Därför bör utvärdering av doser och konsekvenser kunna göras helt med ett perspektiv för att skydda miljön. När SKB har bestämt storleken på biosfärsobjekt så har man ändå utgått ifrån människans perspektiv och inte tagit hänsyn till hur andra organismer använder landskapet och hur stor yta de behöver för att överleva. SKB bör beräkna objektens storlek utifrån de identifierade organismernas hemområden som kan sägas vara ett mått på hur stor yta olika organismer behöver. Se utdrag från BIOPROTA:s rapport 2015, Tabell 2.
6. De högsta dosraterna till organismer beräknades till 10^{-2} μGy h^{-1} i TR-14-01. Då en ändring av ett objekts storlek från ett mänskligt perspektiv till ett miljöperspektiv kan höja radionuklidkoncentrationer med en storleksordning och med de andra ovanstående frågorna i åtanke så bör SKB även uppdatera inventariet av radionuklider i SR-PSU för biota så som man gjort för människa. Eftersom man då kan tänkas beräkna dosrater i närheten av screening-värdet.
7. I ERICA-verktyget kan inte dosrater från inhalation av gaser beräknas. Det finns dock en modell för att beräkna detta (Se t ex Vives i Batlle et al., 2015; Vives i Batlle et al., 2012). Varför har inte SKB använt detta tillvägagångssätt för beräkningar för inhalation? Hur skulle SKB:s beräknade dosrater påverkas av detta?
8. Enligt TR-14-09 har SKB valt CR-värden för olika organismer baserat på vilket ekosystem som de antas vistas i, t. ex. har fåglar och utter i akvatiska ekosystem försetts med akvatiska CR-värden. Detta antagande har dessvärre visat sig kunna resultera i en underskattning av upptaget av radionuklider. Stark et al. (2015) visade i en studie av kontaminerade våtmarker (som kan antas vara en kombination av terrest och akvatiskt ekosystem) från IAEA EMRAS II att just upptaget för en fågel underskattas om den antas äta endast från det akvatiska ekosystemet. Istället gav en kombination av CR-värden en bättre uppskattning och användandet av terrestra CR-värden var mer konservativt. Detta kan gälla även för utter. SKB bör därför se över sina antaganden av CR-värden utifrån detta.
9. I systemet för skydd av miljön från skadliga effekter av strålning är det populationen av organismer som ska skyddas. Hur stor del av populationen av olika organismer kommer att få de av SKB beräknade dosraterna?

Tabell 2. Hemområdens storlek (m^2) för representativa arter av referens organismerna däggdjur, reptil, groddjur, insekt och jordlevande evertebrat: Utdrag och översatt från BIOPROTA (2015).

Namn	Latinskt namn	Hemområde (m^2)
Brunråtta	*Rattus norvegicus*	<9000
Långsvansad skogssork	*Myodes glareolus*	<700
Skogsödla	*Zootoca vivipara*	<1700
Vanlig groda	*Rana temporaria*	500
Större vattensalamander	*Triturus cristatus*	500
Honungsbi	*Apis mellifera*	800
Svartmyra	*Lasius niger*	3
Stor daggmask	*Lumbricus terrestris*	1.6

4. Slutsats

I denna rapport redovisas resultaten av en granskning av utvärderingen av radiologiska effekter på andra organismer än människa i SKB:s långsiktiga säkerhetsanalys SR-PSU. Resultaten visar att SKB generellt använder en internationellt accepterad metod för att beräkna screening dosrater till biota. Beräkningarna resulterar i dosrater som ligger under internationellt rekommenderade screeningdosratnivåer för biota inom strålskyddet av miljön. Dock kan det konstateras att SKB behöver förtydliga och motivera varför vissa antaganden görs i utvärderingen. Som exempel kan nämnas antaganden om biosfärsobjektens storlek som påverkar radionuklidkoncentrationerna i ekosystem media och antaganden om upptag av radionuklider i biota. Förtydliganden behövs för att möjliggöra en bedömning om SKB:s utvärdering av radiologiska effekter på andra organismer än människa är konservativ.

5. Referenser

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APPENDIX 1

Granskade SKB rapporter

Tabell 3: Följande SKB rapporter har granskats.

Granskad rapport	Granskat avsnitt	Kommentar
TR-14-01 Safety analysis for SFR Long term safety Main report for the safety assessment SR-PSU	Främst kapitel 7 - 9	Relevanta delar för utvärdering av radiologiska effekter på biota
TR-13-23 Assessment of risk to non-human biota from a repository for the disposal of spent nuclear fuel at Forsmark	Alla	
TR-14-09 Radionuclide transport and dose calculations for the safety assessment SR-PSU	Kapitel 8	Relevanta delar för utvärdering av radiologiska effekter på biota
R-14-02 Handling of biosphere FEPs and recommendations for model development in SR-PSU	Kapitel 2 och 3	Relevanta delar för utvärdering av radiologiska effekter på biota
TR-14-06 Biosphere synthesis report for the safety assessment SR-PSU	Kapitel 10	Relevanta delar för utvärdering av radiologiska effekter på biota
R-13-46 The Biosphere model for radionuclide transport and dose assessment in SR-PSU		Relevanta delar för utvärdering av radiologiska effekter på biota

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4

Review of handling of Kd-values used for near- and far-field analyses in the safety assessment SR-PSU

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Registration number: SSM2016-1733
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Contents

1. Introduction

This review supports the Swedish Radiation Safety Authority (SSM) review of the Swedish Nuclear Fuel and Waste Management Company (SKB) application for the expansion of SKB's final repository for low and intermediate level waste at Forsmark (SFR). 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 SR-PSU (SKB, 2014a).

SKB indicates that long term safety of SFR is achieved by limiting the activity of long-lived radionuclides and ensuring the transport of radionuclides is sufficiently retarded (SKB, 2014a). Retardation of the transport of radionuclides is enhanced by slow water flow and the sorption of radionuclides on solid surfaces within the engineered system and in the geosphere (SKB, 2014a). Sorption is a generic term for the partitioning of dissolved constituents onto solid surfaces. These surfaces may include engineered materials, corrosion products, and rock and mineral surfaces. In SKB's models of performance assessment for SR-PSU, the cementitious components (concrete/cement/grout), bentonite, and added geological materials (macadam[1]/crushed rock) are included as sorbing surfaces in the near-field or engineered system, while corrosion products and other potentially sorbing surfaces are excluded. In the far-field or geosphere the SR-PSU performance assessment includes the host rock but excludes fracture-related minerals (SKB, 2014a).

Sorption can encompass a number of mechanistic processes, but in performance assessment models, sorption mainly consists of ion exchange (electrostatic interaction) and surface complexation (covalent bonding of aqueous species with surface groups) (SKB, 2014b). For the purposes of SKB's development of distribution coefficient (K_d) values and performance assessment modelling for SR-PSU, sorption as modelled in the near-field and the geosphere primarily includes surface complexation and ion exchange processes (SKB, 2014c). Because of the evolving nature of the mineral composition of cementitious materials as the materials interact with the aqueous phase, sorption in cementitious materials may also include processes such as precipitation and co-precipitation (SKB, 2014d). Surface interactions, such as sorption, between dissolved constituents and solid phases can be complex, particularly in heterogeneous engineered and natural systems, and are sensitive to changes in the chemical and physical environment. Both the solid phase and the aqueous phase have important components that influence sorption. Key solid phase characteristics include mineralogy, surface area, and sorption site density. Key aqueous phase characteristics include chemical factors such as redox (the oxidation-reduction potential of the system), pH, partial pressure of carbon dioxide (pCO_2), concentration of complexing agents, and ionic strength. Details of how these processes may impact sorption are found in previous reviews (Randall, 2012; Bertetti, 2014) and in supporting documents for the SR-PSU safety analysis (Crawford, 2010, 2013; SKB, 2014a,b,e).

1.1. Objectives

The main objective of this review assignment is to assess SKB's quantification and handling of K_d values used in the safety analysis SR-PSU for both near- and far-field (geosphere) radionuclide transport. With the main focus on the near-field, the review (i) examines the experimental support and theoretical understanding needed for

[1] Macadam is a term for angular crushed rock of a specific size range (2-65 mm) containing little or no fine material below 2-mm in size (SKB, 2014e).

selection and justification of K_d values, (ii) identifies radionuclides for which the quantification of K_d values is most important and assesses the quantification of K_d values for those nuclides, and (iii) examines SKB's handling of uncertainties and sensitivity analyses related to K_d values. The review considers geochemical conditions prevailing in the waste forms, near-field, and geosphere.

Several SKB technical reports (as listed in Appendix 1) and other supporting papers and technical reports in the open scientific literature were examined during this review. The information in these reports was used to examine and assess (i) conceptual models for chemical environments and evolution of the near-field and far-field chemistries, (ii) conceptual models for evolution of the cementitious and bentonite barriers in the near-field, (iii) models for estimating the presence and concentration of complexing agents, (iv) implementation of sorption parameters in the performance assessment model, and (v) technical bases for the selection of sorption values.

2. SKB's Approach to K_d Value Development

2.1. Important Radionuclides

The relative importance of radionuclides in a safety assessment hinges on several factors. These factors include the radionuclide's mass and activity inventory in the waste, half-life, dose conversion factor, and its propensity for transport in groundwater (low solubility and high sorption are transport limiting characteristics). As mentioned previously, the sorption (and solubility) of any particular radionuclide is heavily dependent on the chemical conditions of the environment, and its modelled transport is determined by the safety analysis site conceptual model because the conceptual model drives the selection of K_d values. Although performance assessments typically present results for specific radionuclides, sorption properties are determined by the element and its oxidation state (if it is a redox sensitive element). Thus, while Ni-59 and Ni-63 are important components of the waste inventory and safety analyses for SR-PSU, their sorption is represented by the behaviour of Ni(II).

Review of the radionuclide inventory of the low- and intermediate-level wastes expected for the SFR indicates fission and activation products such as Ni-59, Ni-63, Cs-137 and C-14 dominate the radioactivity inventory (SKB, 2014a,f). When radiotoxicity is considered, actinides such as Am-241, Pu-239, and Pu-240 are important, especially after 1,000 yr (SKB, 2014a,f). From an inventory standpoint, wastes slated for the Silo vault dominate the activity and radiotoxicity inventory.

SKB's selection of radionuclides to be included in the safety assessment appears reasonable (SKB, 2014f), but assumptions regarding secular equilibrium with respect to radon and its daughters are questionable in light of the calculated releases of U-series radionuclides at longer times (SKB, 2014f). Sorption of plutonium, uranium, or other radon isotope precursors near or within the biosphere may act as long-lived sources for radon contamination which may substantively contribute to the estimated dose to potentially exposed groups.

For SR-PSU, SKB conducted several performance assessment calculations including those for expected scenarios of repository evolution over time, less likely scenarios such as accelerated degradation of concrete, and residual analyses, which include tests of loss of barrier functionality (SKB, 2014a,f). Evaluation of the results of these calculation cases is useful in identifying potential radionuclides of concern.

Results of the safety analyses for various scenarios in SR-PSU indicate peak doses are dominated by low sorbing or non-retarded radionuclides such as Ni-59, Mo-93 and C-14(organic) (SKB, 2014f). At longer times (>10,000 yr) isotopes of actinides, such as U-238 and Pu-239 and their progeny (e.g., Ac-227 and Pa-231) also contribute significantly to calculated dose (SKB, 2014f). As would be expected, radionuclides with long half-lives are more important near the end of the performance assessment time period. When important repository capabilities are neutralized in the safety calculations, such as in the cases of no sorption in the repository (CCR_B1) or no sorption in bedrock (CCR_B2), the importance of radionuclide retention, even for low sorbing elements, is made apparent (SKB, 2014 a,f). For example, Ni(II), which has relatively low sorption values (SKB, 2014c), is a significant contributor to dose (as Ni-59) for analyses where the near-field barrier is neutralized with respect to sorption (SKB, 2014f).

Based on inventory, radiotoxicity, contribution to dose over the SR-PSU analysis period, and changes in contribution to dose as indicated by various SR-PSU calculation cases, the selection and handling of sorption properties for several elements were identified for more detailed assessment in this review. These elements include actinium, americium, carbon (inorganic and organic forms), caesium, iodine, molybdenum, nickel, plutonium, selenium, technetium, and uranium.

2.2. Methods

SKB models sorption for both the near-field engineered barriers and the geosphere in the SR-PSU (SKB, 2014a). Near-field sorption is represented for bentonite supports and backfill, cementitious materials, and crushed rock material used in conjunction with bentonite for some waste emplacement areas (SKB, 2014a). Sorption data for all three solid types are required to quantify near-field sorption.

Far-field sorption is modelled for the unaltered host rock. SKB's derived sorption coefficient distributions purposely ignore the presence of fracture lining minerals in the subsurface, choosing instead to focus on relatively unaltered rock (Crawford, 2010, 2013). While this approach is likely quite conservative, it is difficult to correlate the expected predominance of fractures contributing to flow paths with the number of fractures that are lined with sorption-enhancing minerals. Thus, SKB has chosen to pessimistically exclude them from the analyses (SKB, 2014a,b; Crawford, 2010).

Because radionuclide sorption values are dependent on both solid and aqueous phase characteristics, SKB has conducted extensive site characterisation and geochemical modelling to develop the requirements for selection of appropriate K_d values in the near- and far-fields (SKB, 2014a).

2.2.1. Approach to estimating geochemical conditions

SKB has conducted a careful and rigorous characterisation of groundwater geochemical conditions at the Forsmark site including quantification of redox, pH, ionic strength, and pCO_2 conditions for various expected water types (Laaksoharju et al., 2008a,b; Salas et al., 2010; SKB, 2010a,b, 2014b; McMurry and Bertetti, 2012). SKB used the site data to develop models for groundwater compositions expected for the different climatic conditions throughout the 100,000 yr period of performance (Auqué et al., 2013). The expected groundwater composition (e.g., pH, redox, and ionic strength) for each climate phase was then used to guide selection of far-field K_d values (Crawford, 2010, 2013; SKB, 2014c).

A similar approach was employed to estimate geochemical conditions of the near-field (SKB, 2014a,d,e,g). Unlike the far-field, where the host rock characteristics remain essentially constant, near-field materials are predicted to undergo a series of chemical and mechanical changes over the life span of the repository (SKB, 2014a,c,d,e). The chemical changes are driven by the effects of changing climate and the effects of barrier and waste package degradation over time as the materials react with groundwater.

SKB has used the characterisation data along with data from SR-Site characterisation (SKB, 2010a) and the modelling of Cronstrand (2007) and Gaucher et al. (2005) to estimate the type and magnitude of geochemical and mineralogical changes for waste packages and engineered barriers. The model results indicate the changes have a profound impact on the mineralogy, surface area, and chemistry of the pore waters for the engineered barrier materials and, in turn, significantly affect the barriers' sorption characteristics. SKB also includes results of models of redox conditions (Duro et al., 2012) and the concentration of organic complexing agents (Keith-Roach et al., 2014). SKB incorporates the effects on sorption from the presence of organic substances that may form complexes with radionuclide species. These organic constituents generally have a deleterious effect on the sorption of radionuclides. The concentrations of organic complexing agents calculated for the near-field are used to reduce the sorption values of certain radionuclides (SKB, 2014c,f). When the individual model results are combined, the conceptual model for near-field geochemical evolution over time represents a multitude of complex features that directly affect sorption and guides the selection of appropriate K_d values.

2.2.2. Selection of K_d values for near-field

For SR-PSU, sorption data pertinent to bentonite are derived primarily from Ochs and Talerico (2004) and includes updated information included in Ochs (2012) and other sources (SKB, 2014c). The K_d data are provided for unperturbed, non-altered bentonite, and are listed in the form of an expected value and estimated upper and lower limit values (SKB, 2014c). The upper and lower limit values were developed in an effort to represent the uncertainties in the sorption data (Ochs and Talerico, 2004). The data are sampled in the performance assessment using a log-triangular distribution with the expected value as the mode (SKB, 2014c,f,h).

Sorption data for cementitious materials are primarily derived from Wang et al. (2009) and Ochs et al. (2011). Sorption values for the cementitious materials are provided for four stages (I, II, IIIa, and IIIb) of cement degradation/alteration, from fresh (Stage I) to most altered (Stage IIIb) (SKB, 2014c). These stages have varying characteristics that impact sorption potential. SKB has used models of cement

degradation and the expected changes in repository conditions to develop a model for the composition of cementitious materials over time (Gaucher et al., 2005; Cronstand, 2007), and incorporates that into the performance assessment model for each waste vault (Figure 1) (SKB, 2014a). Sorption values are sampled according to the expected characteristics of the cement for the given modelled conditions. The sorption data for the cementitious materials are also provided as expected, upper limit, and lower limit values, and are represented as log-triangular distributions in the performance assessment. The sampled values are conditioned for the amount of hydrated cement paste present in different components. The K_d values are also reduced based on the estimated effects of organic complexing agent concentrations for the conditions (SKB, 2014c,f).

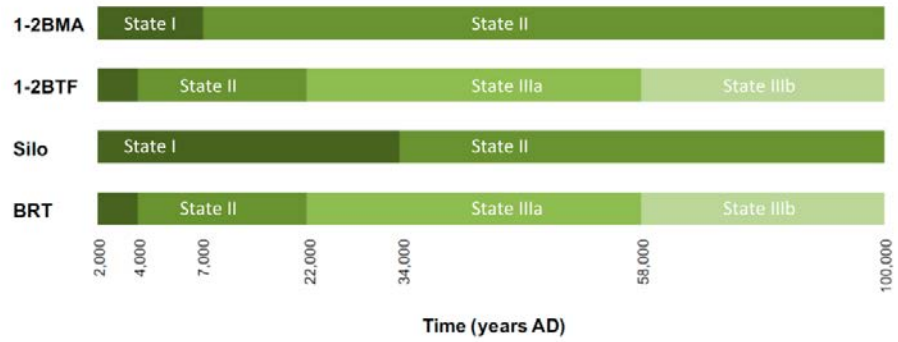

Figure 1. Conceptual model of the evolution of cementitious materials in SFR as they interact with groundwater. The different states (I, II, IIIa, and IIIb) of alteration and their transition times for the various waste vaults are indicated (taken from Figure 7-9 of SKB, 2014a).

2.2.3. Discussion

SKB acknowledges and discusses at length the limited availability of data that can be used for both the bentonite and cementitious material K_d value derivations (SKB, 2014c, and references therein). As a result of the data limitations there is a significant reliance on analogue elements and expert judgment when developing the K_d distributions (SKB, 2014c). Values for some important radionuclides are highly uncertain. Despite comments and recommendations made by SSM and peer reviewers during past reviews (e.g., Little et al., 2012; Randall, 2012; Zhou et al., 2009), there appears to have been little or no progress by SKB in developing any independent pertinent K_d data for SFR. Known data gaps for actinides [e.g., Pu(III/IV) and U(IV)], high radiotoxicity fission products and activation products [e.g., Mo-63 and Se-79), and known low-sorbing radionuclides or those with uncertain sorption mechanisms (e.g., C-14 and Ni-59) have existed for some time and have not been addressed except to modify some upper limits.

A significant advantage of investing in additional experimental work would appear to be development of a more robust safety case with likely improvements in modelled performance. However, it is acknowledged that conducting sorption experiments under conditions relevant to the SFR near-field is difficult and costly, and the expense of these types of activities must be weighed against the value of return of information. For example, it is acknowledged that much of the data for cementitious materials is equivalent to the most recent assemblage available (Ochs et al., 2015), which includes an examination of a very large range of experimental work Additional experimental work that may reduce the uncertainties in the range

of Pu-239 sorption values would reduce uncertainties in the timing of releases of Pu-239, but would likely not significantly change the magnitude of modelled Pu-239 sorption since Pu(III/IV) has consistently shown to be a strong sorber on both cementitious and bentonite materials (Bertetti, 2016; Ochs et al., 2015).

SKB has devoted a great deal of effort to develop a high-quality conceptual model for the geochemical evolution of the near-field (SKB, 2014a). The assemblage of models and site-relevant data provide thorough examination of processes relevant to sorption and produce reasonable estimates of groundwater chemistries over time (SKB, 2014a). The explicit inclusion of models for redox and complexing agents provides a means to update the safety case when additional data are available. SKB's approach to estimating the temporal chemical and mineralogical changes in bentonite and cementitious materials provides a very reasonable basis for selection of K_d values over the repository performance period despite the high, and unavoidable, uncertainties in the specific calculations. One potential area of concern is the degradation of bentonite. SKB notes that there is significant uncertainty in the rate and magnitude of alteration of minerals in the bentonite, as indicated in the widely varying results from different modelling efforts (SKB, 2014c; Gaucher et al., 2005; Cronstrand, 2007). The overall mineral transition sequence appears reasonable, and SKB notes that despite the potential wholesale changes within the bentonite (one-third of montmorillonite transformed after 10,000 yr and nearly all transformed by 100,000 yr) with new clays and zeolites forming (SKB, 2014e), the sorption K_d is assumed to be unchanged over the repository performance period. SKB notes that these replacement minerals will also have high sorption capacity (SKB, 2014c), but there is no support for that statement. Most importantly, the K_d values for bentonite are based on an unperturbed system and are not varied for the duration of the safety analysis period on the basis that the barrier can be expected to represent a homogeneous system (SKB, 2014c,d,e). While other minerals such as zeolites may have desirable sorption characteristics, their response to saline water intrusion or high pH may be different than is modelled for montmorillonite. Additional sensitivity analyses may be warranted to evaluate the use of invariant K_d distributions in the bentonite.

Efforts to calculate concentrations of organic complexing agents and incorporate their effects on radionuclide sorption and transport are commendable (Keith-Roach et al., 2014; SKB, 2014c). Despite the uncertainties in the concentration calculations and the subsequent development of sorption reduction factors, the inclusion of this process allows SKB to evaluate effects on dose for alternate scenarios with higher than expected concentrators of complexing agents (SKB, 2014f). The high degree of uncertainty in applying the sorption reduction will likely remain until additional specific data are available. Unfortunately, the application of the sorption reduction factor seems unclear and inconsistent based on a review of the documentation. Information in the Input Data report (SKB, 2014h) indicates that the reduction factor is applied to bentonite and cement K_d values [Assessment Model Flowchart (AFM) number AFM-118] and alternatively only to cement K_d values (AFM-81). Information in the Data Report (SKB, 2014c) and Modelling Report (SKB, 2014f), which refers to AFM-75, does not clarify the apparent discrepancy in the Input Data report (SKB, 2014h).

The potential for gas formation and its effects on radionuclide transport are also evaluated (e.g., Moreno and Neretnieks, 2013), but the focus is on gas pressure and flow impacts. There does not appear to be discussion of possible effects on pH or barrier degradation from changes in chemistry due to gas development. The addition of H_2 or CO_2 gas may change pH and enhance or degrade sorption. These effects

may be minor or mitigated by the buffering capacities of the bentonite and cementitious materials, but they do not appear to be explicitly addressed in the application documents.

SKB notes several concerns brought forward by SSM during past evaluations (SKB, 2014c). These included a request for stronger arguments that oxidative conditions will not occur after the redox buffering properties of the repository have been depleted. For SR-PSU, SKB supplied model calculations to demonstrate the net reduction capability within the near-field environment for the duration of the performance assessment period (Duro et al., 2012). Another concern pointed to a need for updated retention parameters in bentonite and cementitious materials for several radionuclides including Tc(IV), Np(IV), and Pu(IV) (SKB, 2014c). Unfortunately, no new data appear to have been available to update these K_d values (SKB, 2014c).

2.2.4. Near-Field Sorption Values for Specific Elements

The trivalent actinides actinium and americium are assigned similar K_d values for both bentonite and cementitious materials (SKB, 2014c). There are no available sorption data for actinium, so its selected values are based on analogous behaviour to trivalent lanthanides (e.g., europium) (SKB, 2014c). Sorption values for Eu(III) are also used to supplement americium sorption data (SKB, 2014c). The K_ds for both Ac(III) and Am(III) for sorption on cementitious materials are reasonable and consistent with available data (SKB, 2014c; Ochs et al., 2015). The selected K_ds for both elements for sorption on bentonite are reasonable with exception of the upper K_d limit for Ac(III), which appears to be high based on comparisons to data from Bradbury and Baeyens (2005; 2011).

Sorption of caesium on bentonite is heavily influenced by ion-exchange processes, and alteration of the bentonite in ways detrimental to the sorption of caesium will likely impact (increase) dose at times beyond 20,000 yr (SKB, 2014f). Additional analyses to assess the sensitivity of bentonite degradation with respect to sorption should be considered in light of their influence on caesium transport. The selected caesium K_d values for both bentonite and cementitious materials are reasonable based on a review of available data (Bradbury and Baeyens, 2005, 2011; Ochs et al., 2015).

The inorganic and organic forms of carbon are potentially important contributors to dose (SKB, 2014f). Carbon is likely to be isotopically exchanged or precipitated in reactions with cementitious materials and bentonite porewaters. Because of interferences from organic ligands, SKB conservatively neglects sorption of organic carbon (C-14 organic) for both bentonite and cementitious materials (SKB, 2014c). The selected K_ds for inorganic carbon are reasonable given the uncertainties involved (SKB, 2014c; Ochs et al., 2015). Although the inorganic carbon K_d values are relatively small, removal of near-field sorption capacity (CCR_B1) reveals C-14-inorganic can be a significant contributor to dose without sorption (SKB, 2014f). Additional analyses of the sorption and isotopic exchange of inorganic carbon under repository condition could help to reduce the uncertainties associated with this parameter.

Molybdenum K_d values are selected on the assumption that Mo(VI) is the dominant oxidation state and exists as the molybdate oxyanion (MoO_4^{-2}) (Crawford ,2010; SKB, 2014c). Data exist for the sorption of Mo(VI) on cementitious materials and

are used to estimate K_d values for the engineered barriers (SKB, 2014c). Mo is a redox sensitive element and under anoxic conditions, it can be reduced to Mo(V/IV), but this requires conditions (e.g., high sulphide) that are not expected for SR-PSU (Wang, 2012; Goswami et al., 2012). Data are not available for Mo(VI) sorption on bentonite and an assumed K_d of zero is used in both the bentonite and far-field (Ochs and Talerico, 2004; Crawford, 2013; SKB, 2014c). Based on the data available, the selected values for molybdenum are reasonable and are consistent with the current state of knowledge (Ochs et al., 2015).

Unlike molybdenum, there are substantial sorption data for Ni(II), so its K_d values, though low, are well-constrained, and there is less uncertainty than exists with other low sorbers that lack sorption data (Andra, 2005; SKB, 2014c; Ochs et al., 2015). As discussed in more detail later in this section, use of a log-triangular distribution skews the sampled nickel K_d values low, so dose contributions from Ni-59 may actually be lower than modelled in SR-PSU. The selected values and ranges for nickel sorption appear to be appropriate (Bradbury and Baeyens, 2005, 2011; Ochs et al., 2015).

Although some studies have measured weak sorption of iodine onto bentonite (e.g., Bradbury and Baeyens, 2011), SKB has opted to conservatively model the transport of iodine with no sorption (SKB, 2014c). This appears to be a reasonable selection. Available data for the sorption of iodine on cementitious materials are consistent with the selected ranged of iodine K_d values for the near-field (Ochs et al, 2015; SKB, 2014c)

Selenium may exist in various oxidation states (e.g., VI, IV, and −II) and is likely to be present as Se(IV) under most repository conditions (SKB, 2014a). Although some sorption data exist for Se(−II) (e.g., Iida et al., 2011), the actual presence of Se(−II) under SR-PSU environmental conditions is highly uncertain, and SKB has chosen to model Se(−II) as a non-sorbing element. Similarly, sorption of Se(VI) on bentonite is also set to zero. For Se(IV) the selected K_ds for sorption on bentonite are low, consistent with its measured weak sorption (SKB, 2014c). Se-79 contributes to dose only at very long time frames (>20,000 yr) (SKB, 2014f), which indicates its low K_d value in bentonite is not a particularly important factor. The selected K_ds for Se(IV/VI) for cementitious materials are consistent with available data (SKB, 2014c; Ochs et al., 2015).

For most repository conditions associated with SR-PSU, technetium is expected to exists as Tc(IV) (SKB, 2014a).Tc(IV) exhibits low to moderate sorption in cementitious materials, and the selected K_ds are consistent with the available data (SKB, 2014c; Ochs et al., 2015). K_d values for Tc(IV) sorption on bentonite are selected based on analogous behaviour to Th(IV) (SKB, 2014c). However, data for Tc(IV) sorption on bentonite appear to indicate Tc(IV) sorption is lower than that of Th(IV) (e.g., Grambow et al., 2006; Andra, 2005). Tc(IV) sorption onto bentonite also appears to be influenced by increased in pCO_2 (Andra, 2005). Given these data sets, which suggest an expected Tc(IV) K_d for bentonite of 10 m^3/kg instead of 63 m^3/kg used in SR-PSU, sensitivity analyses should be conducted to evaluate the impact and the need to revise values.

Protactinium is a strong sorber and will be present outside of the near-field only as a progeny radionuclide (e.g., Pa-231) from the decay of actinides (SKB, 2014c). Additionally, there are few data available to develop representative K_d values for protactinium sorption on bentonite or cementitious materials (e.g., Ochs et al., 2015). Based on the available data, the selected protactinium K_ds appear reasonable

(Ochs et al., 2015) and are likely conservatively low for bentonite (e.g., Geibert and Usbeck, 2004).

There are limited data for either Pu(IV) or U(IV) sorption on bentonite, and data for Th(IV) are used to supplement and guide the selection of K_ds for these elements (SKB, 2014c). There are similar data limitations with respect to Pu(IV) and especially U(IV) sorption on cementitious materials (SKB, 2014c; Ochs et al., 2015). While it is likely that these (IV) elements exhibit strong sorption, the reliance on analogue elements to develop K_d values for these radionuclides appears to generate unreasonable uncertainty (SKB, 2014c). Pu-239 and Pu-240 are radionuclides of interest at longer times because of their half-lives and radiotoxicities, and model calculations indicate that plutonium isotopes are significant contributors to dose in some scenarios (SKB, 2014f). Plutonium is also a redox sensitive element and may exist in several oxidation states. Pu(III) and Pu(IV) K_d values for bentonite are linked to results for Am(III) and Th(IV), respectively (SKB, 2014c; Ochs and Talerico, 2004; Ochs, 2012). Recent experimental reviews indicate that Pu(IV) sorption on bentonite may be significantly affected by pH changes (Vilks, 2011), unlike Th(IV), while other data sets suggest that the magnitude of Pu(IV) sorption at higher pH is similar to the SKB SR-PSU expected value (Berry et al., 2007; Amayri et al., 2015; Andra, 2005). Moreover, additional data and a review of the original Th(IV) data (Bradbury and Baeyens, 2003, 2011) appear to indicate that the upper limit K_d for Pu(IV) sorption is too high. Although the uncertainty calculation as applied in Ochs and Talerico (2004) are understood and the upper limit values were reduced previously (Ochs, 2012), there appear to be no reported SFR-relevant Pu(IV) K_d values greater than 300 m^3/kg. Upper limit K_d values for Pu(IV) and U(IV) sorption on bentonite should be on the order of 100 m^3/kg. Similarly, based on data in Ochs et al. (2015) the upper limit for Pu(IV) sorption on cementitious materials should be closer to 300 m^3/kg, rather than the 1000 m^3/kg used in SR-PSU.

In general, there has been a great deal of high-quality scientific work conducted to develop the near-field sorption parameters and the selected K_d values represent the most recent data available (SKB, 2014c; Ochs et al., 2015). Most of this work has been peer-reviewed and evaluated independently. As such, there a few areas of concern with respect to the selected values. Reliance of analogues generates uncertainties for some elements, notably technetium and plutonium. While specific experimental work may help to reduce these uncertainties, the potential changes in sorption values are not order of magnitude changes. For example, Tc(IV) sorption bentonite may be lower by a factor of 5. Sensitivity analyses can be used to determine whether the expense and time of additional work is warranted.

Finally, the use of log-triangular probability distributions, while effective at constraining the lower and upper sampled values, produces median and mean K_d values that are greater than the expected value when the upper limit K_d is much greater than the expected K_d value (mode). This is apparent when calculating the mean and median directly and by inspection of a randomly sampled data set, such as one that might be produced in a performance assessment. For example, expected, upper limit and lower limit sorption values for Pu(IV) on State I hydrated cement paste are 5, 1000, and 1 m^3/kg (equivalent to log K_d values of 0.69, 3, and 0 m^3/kg). Monte Carlo sampling (n=1000) of a triangular distribution, using the log-transformed parameters, produces median and mean K_d values of 14 and 56 m^3/kg for Pu(IV) (Figure 2). The difference in values may be significant for sensitive parameters and does not seem to appropriately reproduce the expected K_d value derived from the experimental data (SKB, 2014f). Additional effort should be made

to constrain uncertainty bounds or modify the K_d distributions to ensure the input data represent intended values. Use of truncated log-normal distributions may be one option. Reducing the dependence on analogues would also help to constrain uncertainty. Separate sensitivity analyses could be used to determine the impact of variations in the upper limits of Pu(IV) and U(IV) K_ds and type of K_d distributions used in SR-PSU.

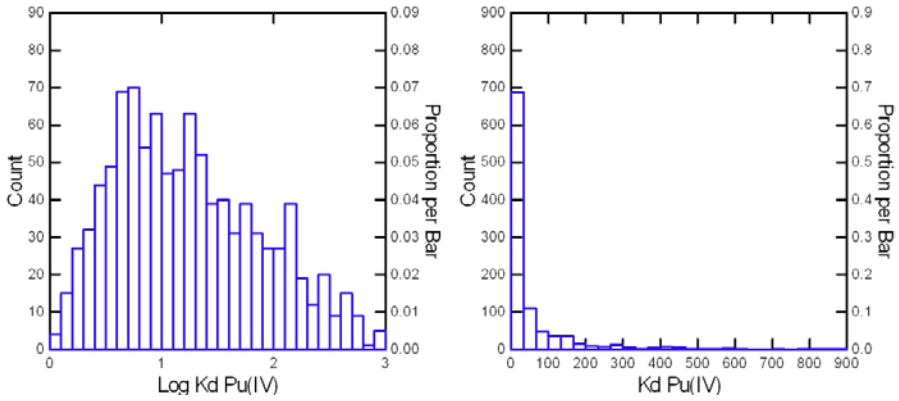

Figure 2. Results of random sampling of a log-triangular distribution with attributes defined for Pu(IV) sorption on State I cement. Because of the high upper limit, mean (56 m^3/kg) and median (14 m^3/kg) sampled values are significantly greater than the expected value (5 m^3/kg) used to define the distribution (and which is representative of the experimental data) (SKB, 2014c; Ochs et al., 2015).

2.2.5. Selection of K_d values for far-field

Sorption data in SR-PSU for the geosphere and rock materials used in the near-field are derived primarily from Crawford (2013), which is an update of Crawford (2010). The approach used to develop these data was reviewed in detail in Bertetti (2014), and this far-field assessment for SR-PSU does not deviate significantly from the findings of that review. SKB notes that the SFR repository environment is geochemically similar to that of the planned KBS-3 repository (SR-Site), and the K_d values in SR-PSU were developed using the same geologic assumptions (SKB, 2014c). The only significant change for development of geosphere K_d data relative to previous safety assessments for the SFR is the addition of K_d values to account for potential high pH plumes from weathering of cementitious materials (SKB, 2014c). Recommended K_d values for radionuclides are given for varying oxidation states and different pH values (less than or greater than 10). The far-field data are provided with mean and standard deviations defining log-normal distributions. The lower and upper limits for the range of K_d values are specified at the 2.5% and 97.5% values for the calculated distribution.

Unlike the approach used for the near-field, the geosphere sorption coefficients are not sampled for temporal or spatial variability, although Crawford (2013) provides varying K_d values for those radionuclides with sensitivity to changes in ionic strength. SKB assumes that the recommended log-normal distribution is reflective of the variability in geochemistry of groundwater, and K_d values are drawn from the lowest provided values that meet the generic criteria of pH<10 and reducing conditions. Sorption values for the crushed rock in the near-field are drawn from the same data set but, where appropriate, values representative of conditions where pH>10 are used.

2.2.6. Discussion

Crawford (2010, 2013) develops K_d values for the geosphere by applying several transfer factors to available experimental data. These factors are designed to adjust the experimental data to scale them for application to the host rock. The transfer factors of Crawford (2010, 2013) are (1) the surface area normalisation transfer factor (f_A), (2) the mechanical damage transfer factor (f_M), (3) the cation exchange capacity transfer factor (f_{CEC}), and (4) the groundwater chemistry transfer factor (f_{CHEM}). Selection of far-field K_d values for SR-PSU utilized the same values for the first three components as was used in Crawford (2010). The f_{CHEM} factor in Crawford (2013) was applied in a similar fashion to Crawford (2010), but new surface complexation modelling was conducted to incorporate new thermodynamic data and to account for the chemical compositions of the different reference groundwater types used in SR-PSU. Crawford (2013) notes that the revised chemistry calculations result in higher K_d values for ion exchangers because, in general, the SR-PSU groundwaters are less saline than groundwaters modelled for SR-Site (SKB, 2010b).

In Crawford (2013) a method is presented to scale the rock matrix K_d values depending on the amount of influence from the repository plumes impacted by high pH from degradation of cementitious materials. This approach, along with a proposed approach to apply K_d values for polonium at various oxidation states, was not incorporated into the performance assessment (SKB, 2014c). As mentioned previously, high pH-oriented K_d values were used for selection of sorption parameters used for crushed rock in the near-field (SKB, 2014c). Uncertainties in the conditions required for the few instances of measured excess poloium activity in groundwater remain large and deciding against explicit incorporation of polonium transport into SR-PSU model seems reasonable.

Crawford (2013) also presents a methodology for scaling sorption on the crushed rock used in the backfill. SKB notes that it agrees with suggestions to use the approach, bur refers to "…Equation 1…without the addition of porosity and density terms" (SKB, 2014c). It is assumed that Equation 1 refers to Equation B-1 in Crawford (2013). However, there appears to be no further explanation of how and when this correction is applied. AFM-75 (SKB, 2014h) lists a data file for other materials and there are several references to the selection and weighting of K_d values for the crushed rock from the far-field value table supplied in the Data Report, but no other details are apparent (SKB, 2014a,c,f).

Inspection of the sorption data for the geosphere suggests that continued application of "pessimistic" selection and conservative approaches may have excessively biased K_d to low values. Even with a two-orders-of-magnitude (factor of 100) difference in available surface area, the expected values for radionuclides such as Tc(IV), Pu(IV), and Np(IV) seem low by as much as a factor of ten (SKB, 2014c). As noted in previous reviews of the far-field sorption data and transfer factors (Bertetti, 2014), the surface area correction used by Crawford (2010) appears to be very conservative and not representative of field data. The relatively insignificant retardation performance calculated in the residual scenarios is likely to be partially driven by artificially low assigned K_d values (SKB, 2014f). As was the case in developing the near-field sorption values, many far-field radionuclide K_d values are derived from analogue elements. For some short-lived and commercially unavailable nuclides, use of analogues may be required because of experimental challenges, but uncertainties for others can be addressed by conducting targeted experiments for site-specific conditions. Again, the difficult nature of these experiments, especially in creating and maintaining solution conditions and verifying radionuclide oxidation states, is

readily acknowledged. But if uncertainties are to be addressed for many important radionuclides, including those with assigned K_d values of zero due to lack of relevant data, some experimental work will need to be conducted.

3. Summary

The methods used by SKB for the development of K_d values used to represent sorption in the near- and far-field for SR-PSU are very similar to established, previously used approaches. In fact, with few exceptions, the methods and resulting K_d values are the same as used in previous performance assessments for SFR 1 and SR-Site (SKB, 2010a, 2014a,c; Ochs and Talerico, 2004). The correction factor and transfer factor approaches used in Ochs and Talerico (2004) and Crawford (2010, 2013) are reasonable, and although the uncertainty ranges are often large, the methods are generally acceptable.

SKB's detailed environmental characterisation and subsequent modelling of various important processes affecting sorption have produced defensible technical bases for expected geochemical conditions in the near- and far-field for SR-PSU. SKB has (i) calculated temporal variation in groundwater chemistry as impacted by climate change and differing hydrologic regimes, (ii) calculated chemical and mineralogical evolution of cementitious materials and bentonite used in the engineered barriers, (iii) modelled the expected redox conditions for the near- and far-field throughout the performance period, (iv) calculated concentrations of sorption reducing complexing agents in the near-field, and (v) applied the results of the modelling and characterisation efforts to guide the selection of appropriate K_d values for modelled radionuclides.

SKB has appropriately identified relevant radionuclides for the transport modelling. SKB has been careful to use pessimistic K_d values for many radionuclides. As might be expected, radionuclides modelled with low or zero sorption tend to dominate the predicted releases of radionuclides to the biosphere. In some cases, low K_d values or K_d values of zero are constrained by lack of data and high uncertainty in sorption behaviour.

Weaknesses of SKB's approach include a continued reliance on analogue data for several important elements, such as plutonium and technetium. In addition, the sensitivity of the SR-PSU results to some elements, such as molybdenum, may warrant further work to evaluate their K_ds. These issues could be addressed by conducting site-relevant limited-scope experiments. However, it is expected that the primary benefit of these analyses would be to improve the performance of the proposed repository by increasing K_ds (as in the case of Mo-93) or by constraining the timing of calculated doses associated with radionuclides with a large K_d range (e.g., Pu-239).

Although SKB's methods for correcting experimental data that may have been collected under differing conditions to determine site-relevant K_d values are reasonable, the application of uncertainty bounds produces upper K_d limits for the near-field that do not appear to be consistent with original and more recent sorption data. The effects of these high upper limits and the use of triangular distributions should be evaluated for their impacts on the representativeness of K_d values. Similarly, although perhaps less important, the far-field K_d values appear to be biased too low as a result of corrections for surface area. A better representation of geosphere performance may be achieved if this correction factor is re-evaluated.

SKB's efforts to develop models for the changes in chemistry and mineralogy of engineered barriers are commendable. However, the model results suggest that the persistence of montmorillonite, or rather, unperturbed bentonite is uncertain. Some analyses should be conducted to provide a better technical basis for assuming similarly effective sorption performance for the altered mineralogy in the bentonite supports and backfill.

The traceability of some model input parameters is not apparent. For instance, how and when the adjustment of K_d values for the presence of competing organic complexing agents occurs is unclear form the available documentation. Likewise, the specifics of apply the scaling factor for sorption on crushed rock materials in the near-field are not available. These discrepancies are relatively minor, but their resolution would provide additional confidence in the SR-PSU calculations.

4. References

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APPENDIX 1

Coverage of SKB reports

The following reports have been covered in the review.

Table A1: List of reviewed SKB reports

Reviewed report	Reviewed sections	Comments
SKB TR-14-01, Safety analysis for SFR long-term safety, main report for the safety assessment SR-PSU	All, with focus on Chapters 2, 4, 5, 6, 7, 8 and 9	Develop understanding of SFR and designed safety features related to radionuclide retardation. Review of modelling assumptions, conceptual model for repository evolution, and results with focus on sorption and important radionuclides
SKB TR-14-02, Initial state report for the safety assessment SR-PSU	Section 3.6, Chapters 7 and 8	Development of understanding of waste vault design and characteristics
SKB TR-14-03 Waste form and packaging process report for the safety assessment SR-PSU	Sections 3.5, 3.6, 4.4, and 4.5	Detailed review of processes and features related to radionuclide sorption and transport for waste forms and packaging
SKB TR-14-04 Engineered barrier process report for the safety assessment SR-PSU	Chapter 2, Sections 3.4, 5.4 and 5.5 through 10.4 and 10.5	Detailed review of processes and features related to radionuclide sorption and transport for different vaults and engineered materials
SKB TR-14-05 Geosphere process report for the safety assessment SR-PSU	Chapters 5 and 6	Review of processes and important features related to sorption and radionuclide transport
SKB TR-14-09, Radionuclide transport and dose calculations for the safety assessment SR-PSU	Chapters 3, 4, and 5, Sections 6.3, 6.4, 6.6, 7.1, 7.2, and 7.4, Appendices A and F	Review of model approach and assumptions, bases for and design of assessment cases, results of specific scenario calculations, and the impacts of radionuclide sorption
SKB TR-14-10, Data report for the safety assessment SR-PSU	Chapters 7 and 8	Detailed review of K_d data development and technical bases for parameter selection

SKB TR-14-11, Model summary report for the safety assessment SR-PSU	Section 3.7 and Appendix A	Review of radionuclide transport model functions
SKB TR-14-12, Input data report for the safety assessment SR-PSU	Chapters 2, 3, 4, and Appendices A and B	Review of actual data sets associated with radionuclide retardation incorporated into SR-PSU
SKB R-13-38, Quantification of rock matrix K_d data and uncertainties for SR-PSU	All	Review of methodologies for selection of K_d values and assessment of uncertainty. Comparison to values from literature sources
SKB R-10-48, Bedrock Kd data and uncertainty assessment for application in SR-Site geosphere transport calculations	All	Re-review of methods and approaches, technical bases for selection of K_d values
SKB TR-04-18, SR-Can, Data and uncertainty assessment, Migration parameters for the bentonite buffer in the KBS-3 concept	All	Review of methodologies for selection of K_d values and assessment of uncertainty. Comparison to values from literature sources
SKB TR-12-12, Assessment of the evolution of the redox conditions in SFR 1	Chapters 4-10, Appendices 3, 5, and 6	Review and confirmation of redox conditions for near-field
SKB R-14-03, Revised assessment of complexing agents in SFR	Chapters 3 and 4	Review of method and technical bases for calculation of complexing agent concentrations
SKB R-13-16, Proposed composition of groundwater for SFR and its extension, during different climatic cases, SR-PSU	Chapters 2, 3, and 4	Review of conceptual model and data used to determine groundwater chemistry, comparison of data with technical bases found in summary reports

APPENDIX 2

Needs for clarifying information

- SKB should provide additional information to describe and demonstrate the application of sorption reduction factors for organic complexing agents to near-field K_d values. The currently available information appears to make conflicting statements about which values are reduced. The application of the sorption reduction factor seems unclear and inconsistent based on a review of the documentation. Information in the Input Data report (SKB, 2014h) indicates that the reduction factor is applied to bentonite and cement K_d values [Assessment Model Flowchart (AFM) number AFM-118] and alternatively only to cement K_d values (AFM-81). Information in the Data Report (SKB, 2014c) and Modelling Report (SKB, 2014f), which refers to AFM-75, does not clarify the apparent discrepancy in the Input Data report (SKB, 2014h). Although this information is unlikely to have an impact on calculated repository performance, it will provide confidence in the calculations.
- SKB should provide additional information to describe and demonstrate the scaling of crushed rock and bentonite K_ds for mixed backfill materials. Crawford (2013) also presents a methodology for scaling sorption on the crushed rock used in the backfill. SKB notes that it agrees with suggestions to use the approach, bur refers to "…Equation 1…without the addition of porosity and density terms" (SKB, 2014c). It is assumed that Equation 1 refers to Equation B-1 in Crawford (2013). However, there appears to be no further explanation of how and when this correction is applied. AFM-75 (SKB, 2014h) lists a data file for other materials and there are several references to the selection and weighting of K_d values for the crushed rock from the far-field value table supplied in the Data Report, but no other details are apparent (SKB, 2014a,c,f). As noted above, the information is unlikely to change the outcome of repository performance calculations but will improve confidence in the results.
- SKB should provide additional evidence or technical bases to demonstrate the use of unchanging K_d distributions for bentonite, given models of chemical evolution that indicate significant alteration is possible. SKB notes that there is significant uncertainty in the rate and magnitude of alteration of minerals in the bentonite, as indicated in the widely varying results from different modelling efforts (SKB, 2014c; Gaucher et al., 2005; Cronstrand, 2007). SKB notes that these replacement minerals will also have high sorption capacity (SKB, 2014c), but there is no support for that statement. One approach to this analysis could be a calculation similar to the bentonite degradation calculation case (CCL_BB) with the addition of loss or change in bentonite sorption values as a result of the degradation.

APPENDIX 3

Suggestions for further in-depth review

- SSM should consider conducting independent analyses of carbon exchange to evaluate the different approaches SKB has proposed for near- and far-field carbon transport. Inorganic carbon-14 is a potentially significant contributor to dose and may have the greatest uncertainty associated with the assignment of K_d values for bentonite and cementitious materials. Inorganic C-14 appears to drive the exceedance of risk criterion at early times in the CCR_B1 calculation case (SKB, 2014f). Additional sensitivity analyses should examine the lower limit of C-14-inorganic sorption needed to ensure adequate repository performance
- SSM should assess the sensitivity of SR-PSU results to bentonite sorption degradation in conjunction with its hydraulic or flow-related degradation over time. SKB notes that there is significant uncertainty in the rate and magnitude of alteration of minerals in the bentonite, as indicated in the widely varying results from different modelling efforts (SKB, 2014c; Gaucher et al., 2005; Cronstrand, 2007). The overall mineral transition sequence appears reasonable, and SKB notes that despite the potential wholesale changes within the bentonite (one-third of montmorillonite transformed after 10,000 yr and nearly all transformed by 100,000 yr) with new clays and zeolites forming (SKB, 2014e), the sorption K_d is assumed to be unchanged over the repository performance period. SKB notes that these replacement minerals will also have high sorption capacity (SKB, 2014c), but there is no support for that statement. One approach to this analysis could be a calculation similar to the bentonite degradation calculation case (CCL_BB) with the addition of loss or change in bentonite sorption values as a result of the degradation. If the sorption potential of bentonite is important for high-activity vaults such as the Silo, then SSM should request or conduct independent modelling of bentonite evolution. SKB's results suggest widely disparate results for their different models, and it would be important to reduce these uncertainties if continued bentonite performance is important.

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Workshop on interdisciplinary aspects of barrier degradation and consequence analysis in SR-PSU

Activity number: 3030014-1031
Registration number: SSM 2017-2170
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Contents

1. Workshop on interdisciplinary aspects of barrier degradation and consequence analysis in SR-PSU

1.1. Introduction

On 19 December 2014, the Swedish Nuclear Fuel and Waste Management Company, SKB, submitted an application to the Swedish Radiation Safety Authority (SSM) for the expansion of SKB's final repository for low and intermediate level waste at Forsmark (SFR). SSM is in the process of reviewing the application.

SKB's assessment of the long-term safety of the repository is documented in the SR-PSU safety assessment. SSM is undertaking a phased review of the safety assessment, which involves an initial review and a main review. As part of the main review phase, SSM organised a workshop on 20-21 June 2017 with consultants undertaking review assignments to discuss interdisciplinary aspects of barrier degradation and consequence analysis in SR-PSU.

Roger Wilmot of Galson Sciences Ltd has been contracted by SSM to review SKB's safety analysis methodology and the approach to quality assurance (QA) in SR-PSU and was invited to the workshop to moderate discussions and prepare a workshop report. This report summarises the key points made during presentations of review findings and during the subsequent discussions.

The workshop comprised an introductory plenary session with presentations on overall issues, a series of three workshop sessions focussing on three main topics, and a final plenary discussion with feedback from the topical sessions. The three main topics were:

- concrete degradation;
- biosphere analysis; and
- bentonite initial state and evolution.

The initial presentations are summarised below and the presentations and discussion of the main topic areas are presented in the next three sections. A summary of the final discussion is presented in Section 5.

1.2. Barrier degradation in the context of safety analysis

Flavio Lanaro (SSM) presented an overview of barrier degradation in the context of safety analysis, including the interplay of external driving forces, radioactive decay and transport characteristics.

There are two main types of degradation affecting the concrete barriers: mechanical degradation and chemical degradation. SKB has identified various potential causes

for each of these types, with the consequent potential to affect the safety functions of low flow through the structures and good retention of radionuclides. SKB assesses the effects of moderate degradation as part of the main scenario and treats accelerated degradation as a less probable scenario. More extreme degradation is considered indirectly through two of the residual scenarios named loss of barrier functions: high water flow and no sorption.

In assessing the potential effects of mechanical degradation, SKB does not consider the structural failure of concrete structures but limits the analysis to the effects of higher conductivity with respect to water and gases. In determining the effects of loading on structures, no account is taken of the waste packages or of the grouting around the waste packages

The principal mechanism for chemical degradation is leaching of portlandite and calcium silica gels within the concrete, leading to an increase in porosity and hydraulic conductivity and a decrease in strength and the development of fractures.

Because of cracks apparent during the operational phase in 1BMA, SKB has changed the design of 2BMA compared to 1BMA and utilises smaller caissons cast in a single operation so as to reduce the extent of shrinkage fractures. Operational phase fractures in 1BMA will be repaired but depassivation through chloride intrusion, carbonation and loss of alkaline buffering due to leaching will all accelerate steel corrosion. Expansion of the steel corrosion products will lead to further fracturing and the hydraulic conductivity may increase by four orders of magnitude within a few hundred years.

The presumed different extent of fracturing within the concrete structures of 1BMA and 2BMA are interpreted as leading to different rates of chemical degradation. Rates of degradation also vary with distance from fractures. Some uncertainties are introduced into the modelling of the chemical evolution through the use of different thermo-dynamic databases.

Similar degradation processes will occur in other waste vaults. The concrete structures are only a significant barrier to flow in 1-2BTF and the rates of mechanical degradation for these are faster than for 1-2BMA. The properties of cementitious materials are also important in the silo and in BRT. The slowest rate of chemical degradation is seen in the silo, and both BTF and BRT are assumed to be fully degraded within 100,000 years.

Mechanical degradation and fracturing can also affect the rock vaults. The extent of fracturing differs between vaults and is limited in vaults that are backfilled. Vaults that are not filled can have a damaged zone extending up to 4m.

1.3. Radionuclide transport

James Penfold (Quintessa) used examples from calculations for 2BMA in a presentation on radionuclide transport and its sensitivity to timing of barrier degradation. These were based on an implementation of SKB's Ecolego[1] model in AMBER[2]. Differences between the two implementations were generally within a

[1] ecolego.facilia.se
[2] www.quintessa.org/amber

factor of two with some differences in behaviour at times of change. These differences were radionuclide-dependent and especially apparent in the case of Ni-59. Less difference was seen when the comparisons were made with revised Ecologo results[3], although highly sorbed radioelements, such as Pu, still showed differences. The dependence of the differences on the assumptions relating to sorption was also shown by good agreement between the AMBER and Ecologo implementations for the accelerated degradation cases, which are based on low or zero sorption.

Studies using the AMBER implementation showed results to be sensitive to:

- model geometry, particularly how diffusion through barriers is represented;
- properties of waste packages;
- conceptual representation of barrier degradation; and
- times of changes in engineering properties relative to changes in the biosphere.

1.4. Concrete degradation assessment

Biswajit Dasgupta (South-West Research Institute) gave an overview of SKB's concrete degradation assessment and its links to other disciplines, with particular regard to 1BMA and 2BMA and differences between these vaults.

Degradation of the concrete has effects on the hydraulic conductivity and the diffusivity. However, because diffusivity changes by less than an order of magnitude, it is a less effective metric for degradation than conductivity, which can vary by several orders of magnitude.

Concrete degradation affects the concrete structures[4] within the BMA vaults and also the grout used to embed the waste within these structures. At the time of installation, the crushed rock backfill[5] around the concrete structures has a higher conductivity than the structures and acts as a hydraulic cage. Degradation of the concrete structures is assumed to be such that the conductivity matches that of the backfill at times beyond 50,000 years. SKB's models assume a faster rate of degradation and increasing conductivity at early times than is indicated by the changes of porosity arising from chemical degradation (using the modified Kozeny-Carman equation and 2D reactive modelling).

SKB has observed fractures in the 1BMA concrete walls and floors during inspections in 2000 and 2011 and plans to add an additional concrete structure outside the existing wall and to grout the floor before placement of backfill. SKB also plans to include inspection and control of concrete structures during construction and emplacement operations. However, SKB's assertion that the differences in design will prevent similar problems in 2BMA is not certain. It is also not clear whether SKB is currently tracking all the relevant assumptions for post-closure safety assessments against the repair plans and verification of restoration,

[3] SKB updated the Ecologo results to address an inconsistency between the original implementation and the documented conceptual/mathematical model for loss of sorption on caissons after cracking.
[4] Reinforced concrete compartments within 1BMA are replaced by free-standing unreinforced concrete caissons in 2BMA.
[5] Termed "macadam" by SKB.

and thus whether the initial state model parameter values are reasonable, e.g. fulfilment of the hydraulic cage in 1BMA.

2. Concrete degradation

2.1. Presentations and discussion

In the session on concrete degradation, there were four presentations:

- Assessment of uncertainties and bounding calculations for near-field flows - Joel Geier (Clearwater Hardrock Consulting);
- Uncertainties in near-field chemistry impacting concrete degradation - Steven Benbow (Quintessa);
- Assessment of SKB's handling and quantification of K_d values – Bo Stromberg (SSM); and.
- A short introduction to the waste in SFR - Åsa Zazzi (SSM).

These are summarised in the following sub-sections. The discussions of these presentations is summarised in Section 2.1.5.

2.1.1. Assessment of uncertainties and bounding calculations for near-field flows

SKB uses different approaches to representing the rock mass in models of the hydraulic system at different scales. The review has noted issues with each of these, relating mainly to limitations in the extent to which alternatives have been considered in the parameterisation of the models.

In the case of the discrete-fracture network (DFN) model, for example, SKB has selected only a small number of realisations for use in flow and transport calculations. The methodology for selection of the DFN model realisations is not clear and the realisations selected do not ensure that the range of possibilities is fully bounded, especially for high-flow cases.

SKB's method for upscaling from the DFN model to the effective continuum model is probably conservative in terms of overall flows, but is considered likely to yield a more homogeneous hydraulic conductivity field and hence a less heterogeneous distribution of inflow to the vaults. This may have consequences for the behaviour of the engineered barrier systems. Similarly, inconsistencies in the way in which the vaults are parameterised in the regional-scale and in the site/repository-scale hydrogeological models could affect how boundary conditions are transferred between the different scale models and hence the relative magnitudes of flows between different vaults.

As part of a review assignment, Clearwater Hardrock Consulting developed a simple 1D representation of the hydraulic system which calculates flows through the vaults that are comparable to flows calculated by SKB using complex 3D models. This simple model provides a reasonable and transparent basis for checking the sensitivity of vault flows to the main components of the hydraulic system. The most significant controls on vault flows in the evaluated system are the properties of the

rock mass (high-transmissivity probabilistic deformation zones (PDZs) or relatively high-conductivity equivalent continuum porous medium (ECPM) blocks). Transmissivities within deformation zones (Hydraulic Conductor Domains - HCDs) also affect flows significantly, but the effect is limited by the overall rock-mass properties, such that combinations of high-transmissivity HCDs and high rock-mass conductivities (or PDZs) could lead to more extreme flows.

SKB's calculations of resaturation times based on an older 2001 model used in SAR-08 (SKB, 2008) lead to shorter resaturation times than expected from newer models and interpretations of the hydrogeological data. Increased resaturation times are one reason to question whether the concrete and bentonite component properties assumed by SKB are adequately realistic, especially at early times.

2.1.2. Uncertainties in near-field chemistry impacting concrete degradation

The initial high pH of concrete passivates reinforcing bars and other steel components embedded in the concrete. Processes that lower the pH or otherwise depassivate the steel could result in higher corrosion rates. Potential processes include extensive anaerobic metal corrosion and the replacement of Ca-bearing solids, such as portlandite, with Fe(II)-bearing solids. The possibility of the latter process to occur was investigated by means of thermodynamic modelling in a review assignment by Quintessa. The review concluded, however, that there is little potential for Fe(II) to replace Ca in cement to any significant extent.

Fracturing of concrete may arise through shrinkage during drying, cooling during groundwater re-saturation, or by mechanical loading. In each case, the consequences are to increase the hydraulic conductivity and effective diffusivity of barriers. These in turn may result in increased leaching of Ca and important chemical components, increasing concrete porosity, and potentially widening fractures. The formation of large-volume alteration products within concrete structures may also lead to further fracturing. Such products include secondary minerals such as ettringite and thaumasite formed from cement alteration, and steel corrosion products arising after depassivation through chloride intrusion along fractures.

The reactions of groundwater with concrete adjacent to fractures act to buffer the pH. Armouring of fracture surfaces could limit this buffering, thereby allowing lower pH groundwater to penetrate further into the fractures, depassivating the steel and leading to increased corrosion and further fracturing. Additionally, the altered physical properties of the fracture-concrete matrix interface and the lower pH environment could hinder sorption and thus affect the transport and retention properties of any radionuclides that are released from the waste form.

SKB has not considered armouring or other couplings of mineral alteration with physical properties in the fracture-matrix system. SSM has tasked external experts to undertake independent calculations in order to determine the potential significance of these effects. The conceptual model for these calculations includes both precipitation on fracture surface and diffusion into the concrete matrix. Calculations included a base case and a series of variants with different diffusivities for the armouring layer, different initial flow rates and different assumptions regarding whether the fracture remains open.

In their review assignment Quintessa and Savage Earth Associates performed calculations which show that fractures in concrete will tend to fill with secondary minerals. If fractures remain open, the diffusivity of the armouring layer becomes a key control on the penetration of lower-pH water. The thinner the armouring layer and the smaller its diffusivity relative to the cement matrix, the further along the fracture will relatively low-pH water penetrate. Low-pH waters are calculated as penetrating about 0.25 metres in 10,000 years, with penetration through a vault wall (0.5m) in 20,000 years or so, and maximum penetration of 2-3 m in 100,000 years. As the cementitious backfill / encapsulant within the vault would still buffer pH around waste, these calculations do not affect SKB's safety arguments; only in the case of a steel container immediately adjacent to the fracture in the vault wall might armouring be an issue.

SSM's calculations showed the formation of brucite ($MgOH_2$) as a component of the armouring layer, in contrast to SKB's calculations of chemical degradation based on similar thermodynamic databases. During discussion, it was noted that the water compositions differed between the two sets of calculations and that SKB do model the precipitation of brucite outside of the concrete structures.

2.1.3. Assessment of SKB's handling and quantification of K_d values

SKB's calculations of radionuclide transport are based on a linear equilibrium approach, based on element specific K_d values for different materials. The justification for this approach is similar to that for other comparable safety assessments and the SKB K_d databases are regarded as reasonable in spite of large uncertainties. SKB appear to have considered all the relevant research results but of necessity there is extensive reliance on expert judgement and the use of analogues for radioelements where there are few data. The justifications of changes in K_d in response to the evolution of engineered barriers and chemical conditions are considered reasonable.

SKB acknowledges the uncertainties associated with specifying K_ds and accounts for them in a probabilistic manner by using probability distribution functions, and an order-of-magnitude type of expert judgement anchored in experimental data (using factors 2, 5 or 10). It is difficult to review some of these judgements, often with vague justification, and wide distributions may conceal uncertainties. There is for example no justification of the use of log-triangular distributions. The overall impression is that conservative values are generally used for the engineered barriers.

Radionuclide retardation in the geosphere is much less significant for radionuclide transport from repository to the biosphere than radionuclide retardation in the engineered barriers. Geosphere K_ds used by SKB are derived from data acquired to support the SR-Site safety assessment for the proposed Forsmark Spent Fuel repository. SKB assumed that the 'transfer factors' used to correct laboratory data to in-situ conditions for SR-Site are also valid for SR-PSU, except that different chemical transfer values (f_{chem}) were specified because the chemical conditions around the SFR repository are different to those in the deeper site. The geosphere K_ds are considered generally conservative, particularly because SKB's approach is based on Ochs and Talerico (2004), which uses porosity data now regarded as outdated. SKB's neglect of sorption on fracture-filling minerals, however, means that retardation by rock matrix diffusion may be over-estimated. Overall, the

geosphere K_ds are not significant in the safety analysis but an increased understanding could increase the margins in the safety analysis calculations.

2.1.4. A short introduction to the waste in SFR

The wastes for disposal in the SFR are low and intermediate level wastes from the operation and decommissioning of Sweden's nuclear facilities. SKB has developed inventories for the wastes already disposed, for projected arisings from operations and for projected arisings from decommissioning. SSM's review of the inventory has identified a number of queries, mainly connected to the decommissioning inventory.

In addition to the radioactive inventory, wastes contain chemical substances that may have an impact, directly or through degradation products, on the long-term safety of the repository. SKB has stated that chemical conditions in SFR do not favour chemical degradation of ion-exchange resins, and also concludes that aerobic and anaerobic microbial degradation of these resins will not occur to a significant extent under the conditions in the repository.

SKB identifies the following as potential complexing agents within the repository:

- low molecular weight organic molecules EDTA, NTA, citrate, oxalate, gluconate;
- degradation products of cellulose (ISA);
- cement additives; and
- degradation products of polymers, bitumen and ion-exchange resins.

Inorganic ligands, e.g. CO_3^{2-}, NO^{3-}, SO_4^{2-} etc. are not considered by SKB who concluded that their complexation properties are not significant under repository conditions. The review concluded that the overall types of complexants considered appeared reasonable but that is was unclear why SKB considered the amounts of these to be conservative.

Waste acceptance criteria (WAC) for SFR 1 are currently under review and those for the extension (SFR 3) are under development. These WAC, which cover topics in addition to the radiological and chemical inventories, are needed by SKB and the waste suppliers in support of decommissioning operations.

The review also concluded that gas generation and waste swelling should be further addressed by SKB.

2.1.5. Group Discussion

The group discussion of the presentations on concrete degradation clarified some of the issues raised and highlighted topics for potential further review.

In the discussion of retardation, the question of what was meant by conservative K_d values was raised. It was noted that lower K_d values (presented by SKB as being conservative) allows radionuclides to be released earlier, when there is greater dispersion in the marine systems and hence lower radiological consequences. This is mitigated somewhat by the assumption that radionuclides are only released from 1000 years onwards. However, this is still before terrestrialisation is complete for the main biosphere object, which occurs more than 1000 years later (2275 years

after the start of the simulations). These conservatisms relating to the biosphere mean that the residual scenario in which bedrock K_d values are set to zero is not necessarily conservative.

It was noted that SKB have made K_d measurements on crushed rock representing the rock matrix. In repository conditions it is expected that fractures are covered by minerals and thus that the measurements might not be very representative for real conditions. Fresh rock should, however, be representative for newly formed fractures in the excavation damaged zone. It was also argued that using values for fresh rock can be regarded as conservative.

It was noted that different waste management programs tend to reference each other and that there is a risk of circular referencing. On the other hand it was noted that data on K_d for concrete is hardly needed for any other purposes, which implies that only radioactive waste management organisations work on this topic. It seems that the Japanese program has put effort into more detailed chemical thinking, factoring in co-precipitation and similar processes to get better K_d parameterisations.

The coupling of concrete degradation and mechanical strengths was discussed. The largest loads can be assumed to arise relatively soon after closure and to decrease over the period when degradation occurs. When degradation has progressed sufficiently to result in a loss of strength the loads will be substantially lower, and this consequence of degradation will have a limited effect on repository performance.

The uncertainties in SKB's hydrogeological calculations were discussed. Given the uncertainties it could well be that the flows could increase one order of magnitude. It was argued that this would not make a big difference for the radionuclide transport, since the transport is relatively fast anyway. Localised flows might have effects on concrete degradation and it was put forward that localised flows should be expected due to the nature of flow through the fractured rock surrounding the repository. A calculation case in which all flow is assumed to be focussed into a single vault could be a reasonable bounding case for localised flow.

The comparison of degradation of 1BMA and 2BMA indicates a significant impact of flow on the degradation processes. The combination of the "accelerated concrete degradation" and "high flow in the bedrock" scenarios gives a calculated dose of 15 microSv/year, whereas the corresponding dose for the main scenario is 7.7 microSv/year. Because the scenario with high water flow represents a higher fractile of the expected flow conditions, and not a specially designed higher flow scenario due to uncertainties in the DFN model or on the climate evolution, the question was raised as to whether this scenario combination represents a realistic main scenario.

SKB has noted that some early measurements of groundwater heads can be questioned, and new interpretations of the hydrogeological data would result in longer resaturation times. There was discussion of the potential effects of repository resaturation being slower and whether there are any important impacts of the resaturation time of the repository other than the degradational aspects. If aerobic conditions do persist, it was considered that there could be effect on the chemistry.

A question regarding the links between hydrogen evolution and near-field chemistry was asked. If water consumption is not balanced by inflow salinity could increase,

which is important for the K_d of some key elements. On the other hand corrosion rates may be very slow.

The issue was raised that SKB did not describe any iterative processes between concrete degradation (chemistry) and flow. It may be the case that the uncertainties associated with any such processes are accounted for through the use of higher conductivities than are derived from the porosity calculations using the Kozeny-Carman relationship. SKB should make this argument explicit if that is the approach they have used.

2.2. Plenary discussion

In the plenary discussion, issues relating both to concrete degradation and other aspects of the assessment were raised, including:

- groundwater flow and geochemistry;
- groundwater interactions with the near-field;
- evolution of the near-field; and
- the overall scope of SKB's analysis

There was discussion about the effect of different DFN realisations on the assumed release point to the biosphere. Although the release points are determined primarily by the location of HCDs, which are modelled deterministically rather than the stochastically treated DFNs, the potential for alternative release points should be modelled. It was also asked if higher flows can be coupled to higher dispersion. It was argued that this coupling was not generally accepted in fractured rock hydrogeology.

The uncertainties in the flow calculations were discussed. SKB argues that the high flow in the bedrock scenario is conservative since the flows through the vaults assume the highest realisation for each vault, which is not realistic. It was, however, argued that if one particular vault is driving the dose, the probability for a high flow for that vault might be higher than for all vaults having high flows. It was pointed out that the high flow scenario shows only small effects of increased flows but it was also noted that SKB's scenario does not couple the higher flows to increased degradation. A comparison of the degradation results for 1BMA and 2BMA seem to show, however, that the flow has an important effect on the degradation rates. The low probability of the combined high flow and accelerated concrete degradation scenario could therefore be questionable if the two processes are not independent.

The groundwater chemistry evolution is discussed by SKB, although the treatment of this evolution, and other topics, is determined to be conservative through expert reasoning. Reviewers noted that such judgements and reasoning can be difficult to assess. It was noted that the role of expert judgement is acknowledged in the general advice to the regulations, but it was also noted that there are different levels of expert judgements that should be coupled to different levels of documentation.

The presence of natural concentrations of elements in groundwater will effectively reduce the K_ds for those elements derived from wastes. The only radioelements significant in the SR-PSU assessment for which this might be important is nickel. As SKB has used site-specific groundwater in the experiments the effect of natural occurrence of species should thereby be included.

It was noted that the risk curve is close to the risk limit but that for non-human biota the curves are far below the screening levels. The likely explanation is that for non-human biota the criteria are aimed at protecting populations whereas the dose and risk criteria for humans are intended to protect persons representative of the more highly exposed individuals in the population.

SKB assumes that, following repair, the 1BMA barrier is assumed to proceed without any unforeseen failure and that concrete barrier failure due to poor construction is not treated as a low probability scenario. It was also noted that the uncertainty regarding concrete degradation is not *what* happens but *why* and *when* and that the effects of concrete degradation are coupled to the evolution of the biosphere receiving the radionuclide release. The 1-2BMA vaults are treated similarly in the analysis and all differences are not accounted for explicitly.

Regarding the question of the impact of hydrogen on near-field chemistry, it was argued that it would be rather simple to make scoping calculations. It was highlighted that the effect of Al and Ti should not be forgotten in such calculations.

The question was raised if SKB has shown a good top-down analysis that identifies important aspects and is coupled to the Research, Development and Demonstration (RD&D) programme. It was argued that the safety analysis is presented in SR-PSU but that indications of how the system is optimised in the safety case are not very clear and that the bigger picture is missing. A sensitivity analysis for different parameters in the consequence analysis is given but this might be distracting, since such an analysis is bound by the models that have been used. SKB could have done more on the topic of model uncertainty. It was noted that SSM could have put more focus on this in its previous RD&D reviews.

It was noted that SKB has not explicitly coupled the flow and chemical concrete degradation analyses. Although SKB's selection of an accelerated degradation scenario was judged to be conservative, there is no explicit cause for the accelerated degradation in SKB's analysis. Furthermore there is no increase in flows, and hence radionuclide transport, out of the barrier system for this scenario. Further iterations of the flow and degradation analysis could have been considered.

Further topics were briefly discussed, as noted below.

- It was argued that the role of complexing agents has been studied for decades and that the values for K_d reduction factors should be fairly reliable.
- The question was raised if non-aqueous phase liquids (NAPL) are part of the waste or could be generated from the waste, but this issue has not been raised previously.
- The issue of potential hot spots of relevant chemicals in the waste and whether these could lead to rapid releases was also discussed. Depending on the existence of correlations between different features, the effects may average out or have safety significance.
- The question of other hazards in addition to the radiotoxicity was raised and it was concluded that these issues are handled by the Swedish environmental protection agency, even if some questions regarding this have been asked by SSM in relation to the WAC.

3. Biosphere analysis

3.1. Presentations and discussion

In the session on biosphere analysis, there were four presentations:

- landscape dose modelling – Ryk Klos (Aleksandria Sciences);
- review of biosphere modelling - Russell Walke (Quintessa);
- implications of SKB's handling of K_d and CR values on consequence analysis results – Laura Limer (Quintessa); and
- SKB's complementary information - calculations about biosphere objects – Shulan Xu (SSM).

SKB has developed a new approach for biosphere and dose assessment modelling in SR-PSU. This explicitly models releases to the biosphere and does not rely on the equilibrium "landscape dose factors" (LDFs) used in the SR-Site assessment. The biosphere is represented by a set of biosphere objects that are based on the location of future lakes and groundwater discharge areas. A landscape model is used to determine the evolution of these objects, based on different climate evolution scenarios. Catchment-scale hydrological modelling, using MIKE-SHE, is used to calculate water flows for use in dose assessment modelling, using Ecolego.

The review of the landscape modelling concluded that the documentation was not of the usual high quality, with key themes difficult to follow through a set of disjointed reports. There was also concern that the mathematical descriptions were written in a non-standard format which made them more difficult to assess.

New features, events and processes (FEPs) were introduced to the modelling (relative to SR-Site) by a FEP analysis, but the implications for the results have not been well documented and the motivation for changing the models was weak. The resulting hybrid model is considered to be overly complex and lacking in adequate justification given the effects on calculated results.

The translation of material from the site descriptive model was not covered in sufficient detail. One example is the conversion of water fluxes from the MIKE-SHE model into water fluxes in the dose assessment model, where there were very different discretisations with around 3.4 m of the lower regolith being ignored with little discussion.

An independent implementation of the biosphere model has been used to review the completeness of the model specification, to verify the results and to develop greater insights into the complex model. Simplifications were used in implementing the model in AMBER and, as particle-tracking asserts that almost all releases are to Object 157-2, the focus was on Objects 157-2, 157-1 and 116, consistent with a reduced version of SKB's Ecolego model that was used in the SR-PSU analyses. Biosphere Object 157-2 is unusual in that it evolves directly from sea to land without a lake stage.

Key differences between the biosphere modelling for SR-PSU and other assessments are the treatment of carbon and use of 50-year average concentrations in agricultural

soils. The explicit representation of carbon pools within the biosphere model, the use of carbon-based diets and assumptions about ^{14}C loss from mire soils all inhibit direct comparisons with other assessments.

The dose assessment model assesses four exposed groups:

- Drained mire farmer
  - grow food on drained mire within one of the biosphere objects, obtain water from dug or drilled well
- Infield-outland farming
  - use of hay from mire within one of the biosphere objects for animals, grow crops with manure, water from dug or drilled well
- Hunting and gathering
  - fishing, hunting, collecting berries and mushrooms from all biosphere objects, obtain water from streams or lakes
- Garden plot household
  - use dug or drilled well, includes irrigation

The infield-outland farming and garden plot groups do not spend any time within the biosphere objects, but make use of potentially contaminated materials.

Although the groups are presented as being "self-sustaining", some are characterised by very low occupancies and food intake fractions. The garden plot householder, for example receives only 8% of their dietary carbon from their produce, and this group and drained mire farmer spend only 54 hours per year in contaminated areas. Similarly, a hunter-gatherer gets less than 0.7% of their dietary C from lake fish in 157-1 and <2% of their dietary C from both 157-1 and 157-2 once they are terrestrialised. None of the other groups are assumed to consume fish, although the consumption of fish dominated the ^{14}C dose in the SAR-08 assessment.

Other observations from developing the AMBER implementation of the SR-PSU biosphere model are that there high loss-rates for ^{14}C (governed by the 'piston velocity' parameter) from mire soils (85 /y) and surface water (20 /y), and very low capture fractions (zero to 0.3%) from drilled wells. Significantly higher capture fractions can be obtained through alternative, plausible assumptions. There are also inconsistencies between the deterministic and probabilistic elements of the biosphere model, for example the way in which in-growth in agricultural soils is treated.

Although complex and extensive, the model description was adequate to allow an independent implementation and the results proved to be close to those in the SKB model. In the case of fluxes from the geosphere, modelled concentrations in the drained mire (the most exposed group) were generally within a factor of 2, with those from the AMBER model generally lower. In the case of calculated doses, results agree within a factor of a few but with the AMBER results now generally higher. The discrepancy here appears to be an error in the Ecolego calculation where the fraction of biosphere object 157-2 that is mire is double-counted.

The AMBER model has been used to explore some specific variants, including lateral connectivity between objects, including the possibility of an impermeable clay layer with enhanced sub-surface flows from biosphere object 157-2 (which receives the groundwater discharge) and 157-1 (which includes a lake). Further variants may arise from alternative conceptualisations using recently released information from SKB.

Results can be difficult to interpret because the model is a hybrid of deterministic and probabilistic modelling. It is, however, easy to find interpretations that are

plausible and which could give rise to higher doses. The model for ^{14}C in the system is new. The old model (used in SAR-08; SKB, 2008) is known to be rather simplistic and conservative and this is the justification for the new model having been developed. There are, however, several parameters within this model that appear to be non-cautious.

The overall conclusion is that the biosphere model as documented cannot be said to provide a conservative estimate of potential impact. The interpretation of the reviewers is that the biosphere modelling is an attempt to provide a realistic rather than cautious description of the FEPs in the biosphere that would give rise to exposure and as such does not give a full indication of the potential radiological impact of the repository.

SKB has used a highly automated process of extracting site-specific data from SKB's data archives, and using these to calculate and 'quality assure' K_d and concentration ratio (CR) values. This is highly complex and not well documented in the original reports. The process was ultimately traceable with the aid of further explanatory documents.

The eventual statistical power of the site-specific parameters obtained is limited by low numbers of data pairs from which K_ds and CRs can ultimately be calculated (e.g. N=7 for K_d RegoLow for nickel; N=1 for CR for nickel in fish). Methods applied to compensate for this lack of statistical power, including the use of the statistical variation of ALL elements to represent plausible variation in a parameter for a single element seem arbitrary. SKB concedes that the process of defining the plausible limits of CRs and K_ds is "to some extent subjective and based on the general assumption that it is conservative to widen the PDFs of selected parameter data".

Further review of SKB's datasets for K_ds and CRs has compared data used for SR-Site and SR-PSU. The different waste inventories between these repositories require the derivation of data for elements not considered in SR-Site. In SR-PSU, SKB has made quite extensive use of element analogues (e.g., nearest-neighbours in the periodic table) for deriving these data. Qualitative similarity in the chemistry of an element and its analogue, however, is no guarantee of a quantitative similarity in parameter values for K_d and CR. The review concludes that several of the selections of element analogues in SR-PSU have involved choices which are not particularly well justified.

The implications of SKB's selection of K_d and CR values for the consequence analysis are not immediately clear as some changes to the distributions will lead to higher calculated doses, and others will serve to reduce the calculated doses. Further, to fully assess the uncertainties in these parameters, consideration should also be taken of their behaviour in the near field and geosphere at the same time.

During the initial review phase, SSM noted that SKB's central calculations in SR-PSU are based primarily on radionuclide releases to a single biosphere object 157-2 and that these do not reflect uncertainties in the modelling of landscape development. SSM believes that biosphere modelling and dose calculations should be conducted to provide a series of outcomes that cover reasonable future scenarios. SSM therefore requested additional information that illustrates the uncertainties regarding different types of objects, such as by reporting radionuclide release directly to a biosphere object that is a lake.

In response to this request, SKB submitted further calculation results, based on:

- alternative landscape evolutions, with a lake in object 157-2;
- an alternative realisation of the fracture network, which leads to discharge to three objects including two lakes; and
- sensitivity analysis of discharge points/areas affecting environmental media concentrations and doses.

3.2. Plenary discussion

SKB's treatment of carbon in the biosphere was discussed and a specific question asked about root uptake. Such uptake is very small and SKB has modelled it differently compared to previous safety analyses.

The differences between the biosphere analysis for SR-PSU and that for SR-Site were discussed as the two are quite different. It was noted that for SR-Site the biosphere is not a very important issue since the calculated risk is far from the risk criterion. For SR-PSU the calculated risk is close to the risk criterion and SKB has striven to be realistic and has made large efforts to be able to underpin assumptions that lead to lower ^{14}C dose consequences.

In most assessments internationally the exposed groups include subsistence type farmers, which imply a cautious set of activities compared to what people usually do and thus can be argued to be stylised. SKB has moved away from this and made more realistic assumptions for the biosphere. This may have implications for the treatment of the geosphere and whether the different modelling assumptions regarding groundwater flow and transport are appropriate.

4. Bentonite initial state and evolution

4.1. Presentations and discussion

In the session on bentonite, there were two presentations:

- Uncertainties in bentonite initial state and mechanical evolution and its links to other disciplines - Göran Sällfors, Geoforce; and
- Uncertainties in bentonite (montmorillonite) degradation and its links to other disciplines - Mick Apted, Interra.

SKB's design for SFR uses bentonite in three forms: as blocks, as pellets and mixed with sand. In each case, two key properties are swelling pressure and hydraulic conductivity and these may be affected by the degree of saturation and swelling, by piping and other erosion processes, and by freezing. The key safety functions of the bentonite are:

- to limit water flow through the waste packages; and
- to retard outward transport of radionuclides from the repository by, *inter alia*, sorption.

The principal processes affecting the safety function of the bentonite are shown in Figure 1. For the backfill and plugs, the main issue is construction & installation, i.e. can it be built as designed? The plug installation and tunnel sections to be

backfilled with bentonite are sensitive to larger point inflows. SKB therefore intends to grout the rock mass where major point flows have been observed. SKB also mentions that if necessary they can wire-saw the rock mass around the plug positions to decrease the excavation-damaged zone (EDZ). SKB estimates that the same criterion used for the spent nuclear fuel repository[6] for an accepted total inflow of <10 *l/min* per tunnel can be seen as a threshold where no special efforts are required to remedy the inflow of tunnel sections to be backfilled with bentonite in SFR.

The review concludes that the initial values of hydraulic conductivity and swelling pressure used by SKB in the safety analysis are reasonable, based on the density of the bentonite in various parts of the repository. However, SKB needs to demonstrate that they can construct and install the bentonite so that it achieves the presumed initial state. .

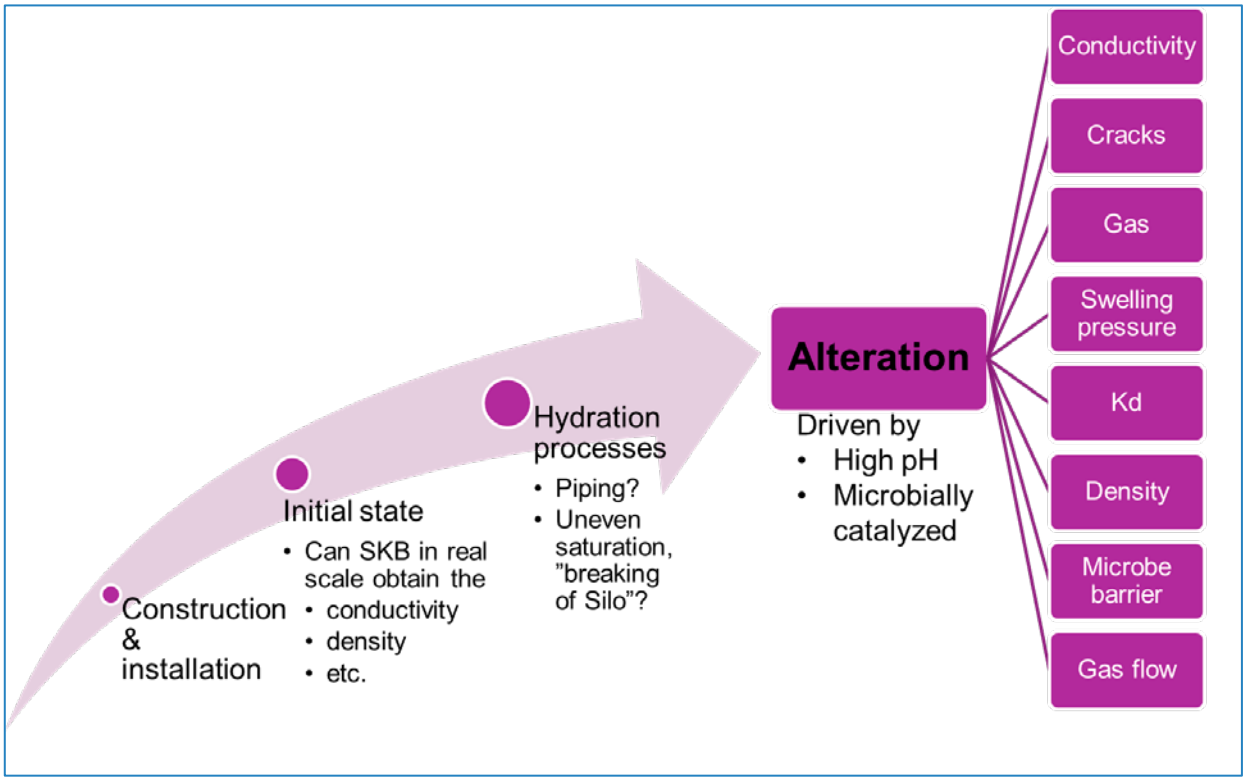

Figure 1. Flow-chart showing construction, installation and internal processes affecting the barrier functions of the bentonite. Are all of these different factors included in SKB's FEP database? Note: not included in the flow chart are external factors that can affect the barrier functions (freezing and chemical erosion).

Figure 1 omits freezing and chemical erosion as processes that could affect bentonite performance. The review concurs with SKB that freezing can be considered as a less probable scenario, based upon the fact that permafrost occurs relatively late and there are still uncertainties concerning the freezing depth. Bentonite can be expected to be fully saturated by that time and hence its mass will be relatively evenly distributed.

[6] For inflows, SKB proposes a level of 10 litres per minute per 100 meter tunnel length as being acceptable (SKB, 2010).

The review also agrees with SKB that chemical erosion is unlikely to occur and that even if it does occur, its impact on safety will be small. This judgement is based on:

- cement close to the bentonite can provide sufficiently high Ca^{2+} concentration for a very long time (chemical erosion is a colloid chemical process);
- glaciation occurs at a very late stage even with the climate case of glaciation; and
- at the time of glaciation and potential chemical erosion the radioactive inventory will be several orders of magnitude lower than the initial activity.

Figure 1 shows that many properties of the bentonite may be affected by alteration. The two main types of alteration that could potentially occur are:

- microbially catalysed transformation of montmorillonite to illite; and
- high pH dissolution of montmorillonite followed by precipitation by zeolite, silica, illite etc.

These mineral transformations result in reaction products that have different properties to bentonite, for instance no swelling in the presence of water. This will affect the barrier mechanical, hydraulic and chemical barrier functions.

Microbially catalysed transformation of montmorillonite to illite has been shown to occur in experiments, but the experimental conditions (standard room temperature and pressure, material in suspension) are very different to the in situ conditions. It is very uncertain if such alteration can or will occur in repository conditions, particularly at early times. However, it is open for discussion if this qualitative assessment needs to be confirmed quantitatively.

In the case of high pH alteration, it has been shown by mass transfer and chemical kinetics calculations that the alteration depth in the bentonite is rather shallow, ca 10 cm (Savage et al., 2010, Table 8). The propagation of the alteration front is inhibited by the previously altered zone. SKB's approach is to apply only the assumption of a mass transfer limitation and not a limitation for chemical kinetics. Thus, the review considers that SKB's approach is conservative.

SKB has published a report (SKB, 2016) on the long-term performance of the bentonite in the silo (which contains some 70% of the disposed activity) but this had not been reviewed to date.

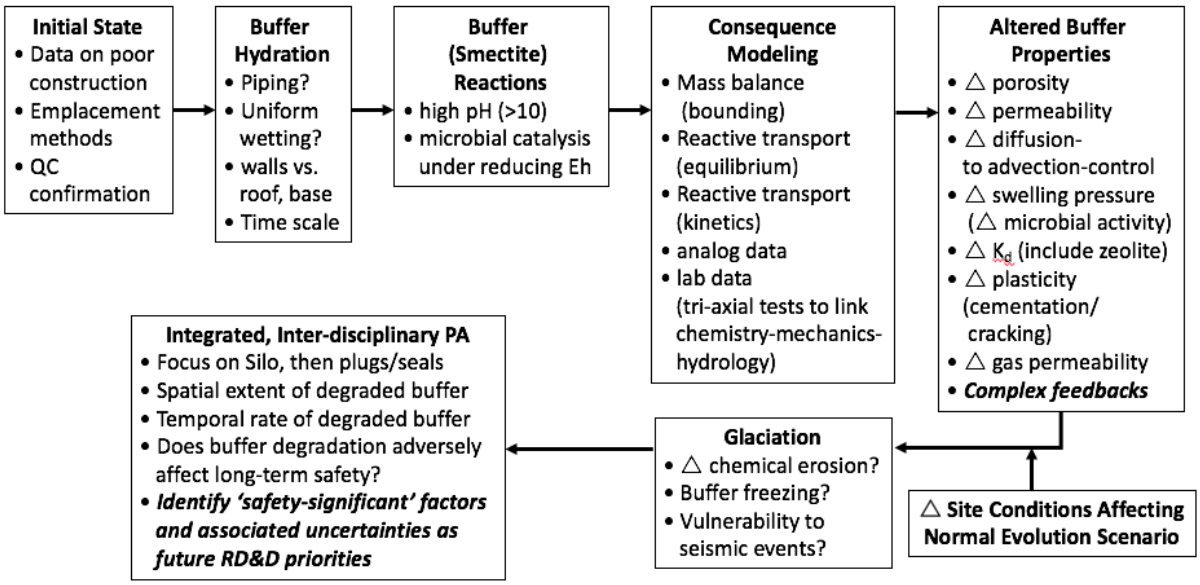

Figure 2. "Storyboard" for buffer alteration effects on long-term SFR safety

Figure 2 presents an integrated 'Storyboard' of the range of topics discussed regarding the uncertainties related to potential degradation of the montmorillonite (smectite) component of bentonite buffer used in various parts of the SFR repository. The "Δ" symbol denotes '*change in properties*', so, for example, *"Δ porosity*" means the topic of potential change in porosity of buffer from postulated changes arising from smectite alteration/ transformation.

Based on this 'storyboard' review and summation, in which different scientific and engineering disciplines were jointly considered, key messages include:

- based on available evidence and conditions expected for the SFR, it seems unlikely that safety-significant amounts of montmorillonite in buffer will be altered over regulatory time scales of concern, thus preserving the intended safety function;
- as part of a performance confirmation program to further enhance regulatory confidence, there may be opportunities for SKB to more strongly link chemical-mechanical-hydrological changes in buffer properties using innovative test apparatus, possibly tri-axial cells; and
- SKB ought to identify 'safety-significant' factors and associated uncertainties from current process models and integrated performance-assessment models in order to provide a guide and defensible basis for future RD&D priorities.

4.2. Plenary discussion

Although microbial transformation of bentonite can be very fast under conditions that are optimal for the microbes, such conditions do not prevail in the repository and this type of alteration is not considered important. It is, however, an example of where SKB's FEP list may not be complete. Reviewers noted that processes such as this should be identified and then screened out rather than simply being excluded.

SKB's assumption that there will be little microbial activity at the pH values within the repository also means that the microbial gas generation rate will be low. Higher gas production rates could become an issue if microbial activity is high for any reason.

The importance of the initial state of the bentonite was discussed. The silo has already been built and thus the emplacement of the bentonite has already taken place. The initial conditions for the long-term safety analysis also include the manner in which the bentonite re-saturates. Swelling and movements of the bentonite are measured and sinking of the silo has been observed due to the emplacement of waste. The measurements have so far matched well to the modelling results, although water content measurements often have failed. In order to prevent re-saturation in the silo during operations SKB has covered the rock walls with shotcrete and installed a drainage system. When the drainage system is shut down, the bentonite is expected to be saturated from the bottom to the top. SKB proposes similar techniques in other areas, potentially with the inclusion of plastic sheets in some places.

Although bentonite emplacement around the silo has already taken place and would be difficult to change, there are measures that could be taken during further operation, e.g. limitations to deposition of waste, repairs or removal of waste, even if it was considered unlikely that waste already grouted would be retrieved from the silo. Thus it is meaningful to give attention to the silo, both currently and in association with the required re-evaluation of safety every ten years. It was noted that a near-field transport model of the silo would be a work intensive task to implement.

One of the less probable scenarios assessed by SKB is based on bentonite degradation. In this case, however, it is the hydraulic properties of bentonite that are assumed to be degraded and sorption is assumed to be the same as for the intact bentonite scenarios. It was noted that there is no data to underpin this assumption of degraded bentonite having equal sorption characteristics to intact bentonite but it is a common assumption in other programmes. NAGRA has done some work but only on alteration of pH conditions and not on mineral transformations. SKB does assess the effects of zero sorption in bentonite by means of the residual scenario *loss of barrier function scenario – no sorption in the repository*.

The potential for flows through the repository to be higher than assumed by SKB was discussed. Although the effect of higher flows on bentonite degradation was judged to be small, higher flows in the main scenario would imply higher flows in the other scenarios in which there was barrier degradation. It was noted that flows could be higher in particular vaults and also that the aggregated flows could be higher due to the way the flow cases have been selected by SKB. This selection is based on the summation of the transmissivities of fractures cross-cutting the vaults and thus neglects the effects of the connectivity of the fractures. The results show that most realisations give summed transmissivity values that are rather close together and the effect of different connectivities could therefore affect the aggregated flows. The extent of these differences is difficult to determine without further analyses involving the connectivity of the fracture system, but realisations with better connectivity are likely to exist. It was also noted that two variants of the DFN regarding coupling of transmissivity and fracture size were analysed but that SKB only propagated one of these in further analyses.

The possibility of SKB developing an alternative barrier solution for the 2BMA with a concrete and bentonite system was raised. However, it was questioned whether there is an incentive to optimise 2BMA given that 1-2BTF and the sum of 1-5BLA give higher consequences in some instances than 2BMA. This depends on whether there are requirements to optimise components of the repository.

5. Overall comments

The issue of cautiousness versus realism in the safety analysis was discussed. Reviewers noted that SKB has not clearly stated which parts are cautious and which are realistic. From the radionuclide transport perspective some extreme assumptions and analyses based on bounding cases would encompass a cautious analysis. However, between cautious / extreme and realistic cases there could be cases with significant consequences that have not been explored in detail and it may be these that determine the extent of the safety margins.

The silo and 1BMA had been the focus of discussions at the workshop, but it was noted from the risk curves for the intrusion wells scenario that other vaults also give significant doses. Although calculated consequences from some scenarios are close to or above the risk criterion, in general the calculated doses for SFR are still fairly low in comparison to those reported in SR-Site. Thus it can be argued that the system is not as quality critical as the KBS-3 system.

Reviewers found that the understanding of the disposal system is not as well documented as for SR-Site. SKB's overall application includes a range of studies and assessments in addition to SR-PSU but, in the context of the safety analysis, there is no overall summary of key arguments (a safety case) that can be used to explain the repository functioning to the layman. Discussion of best available technique and optimisation is important in such a safety case.

Usually, every design starts with a design basis and the design is not fixed, even if codes are followed. There are always uncertainties that need to be explored. SKB has not quantified uncertainties in the design and no uncertainties have been propagated. The risk curve is thus a fuzzy line, since some uncertainties are considered within the model, but some inputs are treated deterministically, e.g. flows, even if they also are subject to uncertainties. Scenario and parameter uncertainties are mixed together. It still needs to be demonstrated that 2BMA behaves as intended regarding the initial state; the effects of a lack of knowledge or of a mishap in the initial state of systems are not included in the assessment.

Regarding the DFN it was concluded that SKB relies on the given methodology and the same is the case for the RN-transport analysis. There are oddities in the implementations and there are many conceptual modelling choices. Some of these choices are explored in less probable scenarios, but they are mostly not looked at with different conceptual models.

Some of the less probable scenarios explore the effects of specific events and processes, although the probability assigned to these may be arbitrary. The residual scenarios have a role in analysing the effects of conceptual uncertainties, although these scenarios are based on the loss of safety functions without any specific events or processes leading to such losses. The high inventory scenario is defined as a less probable scenario, with activities based on the 95th percentile values for each

radionuclide in each waste vault. The uncertainty distributions used take account of measurement errors and correlations but not in the amount of waste. Use of the 95th percentile values for all radionuclides is arbitrary and no probability can be attached to this scenario. If included, it was suggested that it should be defined as a residual scenario or as a sensitivity study.

In a concluding discussion session, the external experts contributing to the main review phase of SSM's review of SKB's safety assessment SR-PSU were asked to summarise their main conclusions and to identify what the next steps for the review might be.

All of the calculations of radionuclide transport through the barrier systems and the consequent doses are dependent on the actual source term and the release mechanisms of radionuclides from the waste form. These assumptions are not described very clearly and hence there are questions in relation to the inputs to the radionuclide transport calculations. SKB could be asked for additional documentation on these topics.

Sorption is a key process in the assessment of the post-closure performance of SFR. Because early releases from SFR may lead to greater dispersion in the marine systems, SKB's cautious approach when there are uncertainties, and the assumptions made in adopting this approach, can make it difficult to interpret the assessment results. SKB could be requested to present results from calculations based on more realistic assumptions.

SKB's assessment of post-closure safety is dependent on the assumptions they have made relating to the initial conditions of the disposal system at the time of closure. There are concerns as to whether SKB can accomplish such initial conditions in practice. One area of particular interest is the evolution of the bentonite around the silo, the wetting procedure, and the consequent effects on swelling, movement and the equalisation of densities.

SKB does not explicitly consider uncertainties in the design or in the initial conditions. SKB could be asked for further information on the uncertainties associated with the design, how they expect to achieve the assumed initial conditions, how they will manage deviations from the assumed behaviour. The last of these is related to the degradation cases selected for analysis. SSM's modelling capabilities could also be used to explore different degradation cases so as to identify any additional cases that are significant.

SKB's assessment of doses is highly dependent on the location of releases into the biosphere and this, in turn, is dependent upon the selected realisation of the DFN model. Alternative assumptions on the location of releases, and on the interpretation of biosphere objects around the area of release, could lead to different calculated doses. Concerns relating to the location of releases are exacerbated by uncertainties in the behaviour of some of the most significant radionuclides and by the treatment of ^{14}C in the biosphere. There are also errors and QA problems associated with the biosphere analysis, arising in part from what seems to be an overly complicated analysis. Reviewers do not disagree with the fundamental understanding of the biosphere, but with SKB's implementation of the processes.

SKB could be asked for further information and calculation results relating to releases and consequence calculations. Alternatively, because SSM has the capability of undertaking comparable biosphere calculations, alternative assumptions could be tested independently. These could be linked to other elements

of the PA, such as the DFN model, to explore the overall bounds of the assessment and which factors are dominant. Independent calculations exploring the effect of different release points, different exposure groups and different assumptions about biosphere processes would all help build confidence in SKB's results. These results are otherwise difficult to interpret in terms of the degree of cautiousness involved, and hence the overall significance of calculated consequences that are close to the risk criterion.

6. References

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6

Review of Safety Analysis Methodology in SKB's Safety Assessment SR-PSU: Main Review Phase

Activity number: 3030014-1022
Registration number: SSM2016-3953
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Abstract

This review has considered specific issues concerning SKB's methodology for post-closure safety analysis in the SR-PSU safety assessment: (1) FEP handling in the context of deriving the main scenario for the reference evolution of the repository; (2) the assumptions and modelling treatment of gas formation and transport, including the methods for scenario selection used for the identification of the most important course of events; (3) the method for risk summation; (4) the handling of risk dilution; (5) the treatment of uncertainties in the initial state of the barriers and possible malfunctions; (6) the identification of design basis cases; and (7) the reasonableness of the assumptions made and the resulting calculated doses for the future human action (FHA) scenario cases.

The derivation of the main scenario was reviewed through a series of spot-checks of the FEP Report and associated FEP database. These demonstrate that SKB has taken a methodical approach to establishing the relationships between FEPs from a number of sources, but the summary descriptions in the FEP database are not always sufficient to fully understand how a FEP has been treated. SKB's terminology regarding those FEPs that can reasonably be excluded from models is not always clear. A more consistent terminology must be applied if the treatment of FEPs throughout the assessment is to be understood.

Gas pressure build-up in the repository has been assessed by SKB and found to be of insignificant concern. However, this is based on an assumption in the safety assessment calculations that only corrosion of metals contributes to gas formation. In fact, there is significant uncertainty on how much gas might be generated by microbial degradation of organics, and the total volume could be a significant fraction of that generated by corrosion. Given the uncertainties, it would be appropriate to consider a scenario, or at least sensitivity studies, in which methanogenesis is active, and therefore there is a potential for release of C-14 from the repository in a gas phase.

SKB's approach to risk summation is conservative, and is well suited to comparison against regulatory performance measures. However, it not possible to use such an approach for optimisation studies.

Risk dilution is considered by SKB with regard to the earthquake and well scenarios, but its potential importance is not explicitly considered with regard to the treatment of parameter value uncertainty in the probabilistic calculations for other scenarios.

Overall the approach to treating uncertainties in the initial state of the barriers is adequately described. Design basis cases have been identified based on a set of less probable and residual scenarios. The residual scenarios do not contribute to SKB's overall assessment of risk, but they do illustrate barrier significance.

The key assumptions underlying SKB's conclusions regarding the potential consequences of drilling into the repository are subject to significant uncertainties and further calculations are required.

Contents

1. Review of safety analysis methodology in SKB' safety assessment SR-PSU – main review phase

1.1. Introduction and background

On 19 December 2014, the Swedish Nuclear Fuel and Waste Management Company (SKB) submitted an application to the Swedish Radiation Safety Authority (SSM) for the expansion of SKB's final repository for low-level and intermediate-level waste at Forsmark (SFR). SSM is in the process of reviewing the application.

SKB's assessment of the long-term safety of the repository is documented in the SR-PSU safety assessment. SSM is undertaking a phased review of the safety assessment, which involves an initial review phase and a main review phase. The initial review phase, undertaken in 2015, served to develop a broad understanding of the application, to judge whether the application is complete, and to identify key topics for the main review phase. The objective of the main review phase, currently underway, is to undertake more detailed review of particular topics identified as meriting further consideration as part of the initial review phase.

Galson Sciences Ltd (GSL) has been contracted by SSM to review SKB's safety analysis methodology in SR-PSU as part of both the initial and main review phases:

- The results of the initial review of safety assessment methodology are reported in [1]. The initial review focused on SKB's handling of features, events and processes (FEPs) in the assessment, the use of safety functions to structure and communicate the assessment, the approach to scenario development and selection, and the handling of uncertainties in the assessment.

- This report presents the results of the main review phase of SKB's safety analysis methodology. The topics to be considered in more detail during the main review phase were identified by SSM, based on work carried out during the initial review phase by SSM, GSL and others.

1.2. SKB's safety analysis methodology and review topics

SKB's approach to safety analysis includes ten steps, from an analysis of FEPs to dose calculations and evaluation with regulatory criteria (Figure 1). The initial review of SKB's safety assessment methodology focused primarily on Step 1 (FEP handling), Step 5 (Definition of safety functions) and Step 8 (Selection of scenarios). It also considered how SKB had handled uncertainties in all parts of the assessment and the identification of future research needs.

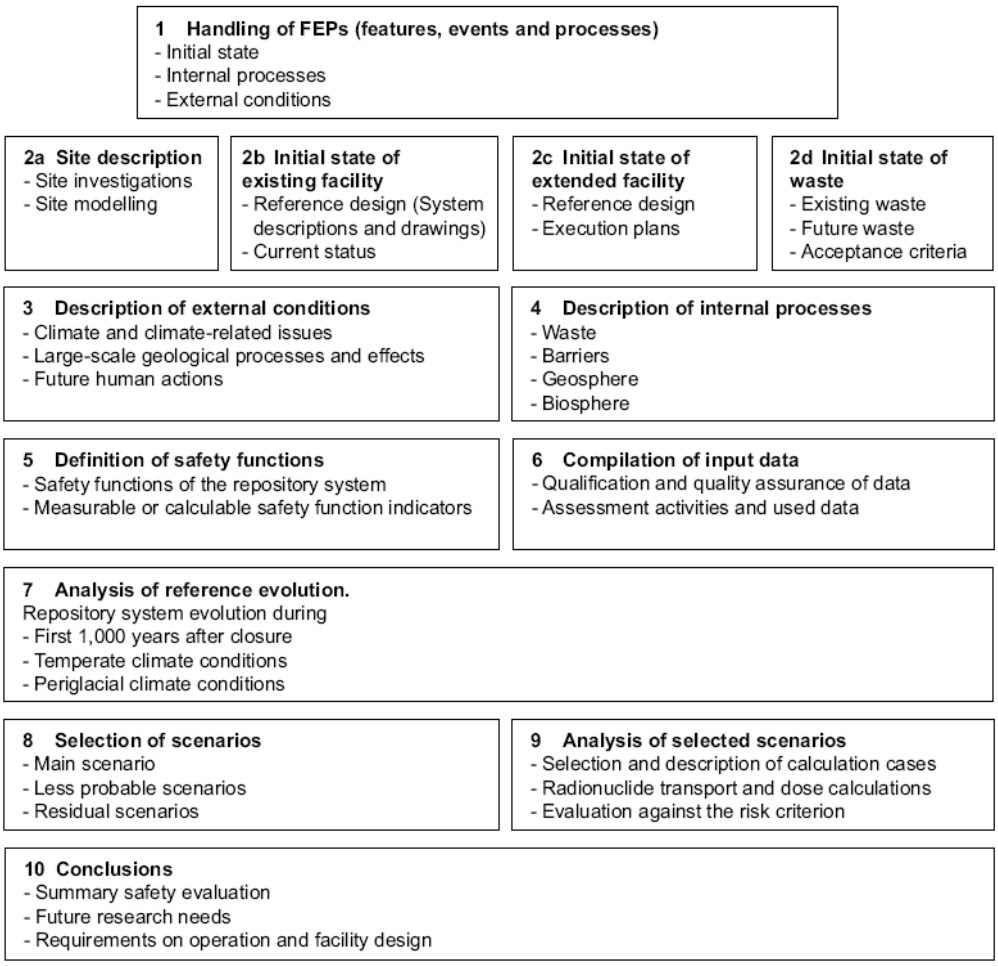

Figure 1 Overview of the ten steps in the methodology used for the long-term safety assessment SR-PSU (Main Report, Figure 2-4).

This report considers the following topics identified by SSM:

1. The derivation of the main scenario for the reference evolution of the repository – Steps 1 and 8.

2. The assumptions and modelling treatment of gas formation and transport, including the methods for scenario selection used for the identification of the most important course of events – Steps 1, 2, 4, 5, 6, 7, 8, 9 and 10.

3. The method for risk summation, and the handling of risk dilution – Step 9.

4. The treatment of uncertainties in the initial state of the barriers and possible malfunctions, and the identification of design basis cases – Step 2, 5 and 8.

5. The reasonableness of the assumptions made and the resulting calculated doses for the future human action (FHA) scenario cases – Steps 3, 6, 8 and 9.

This report of the main review phase therefore provides further consideration of specific aspects of Steps 1, 5 and 8, but also considers issues forming parts of the other Steps. It provides a fuller snapshot across SKB's analysis methodology.

This report is structured to address these five topics[1]. It supports the work reported in [1], and assumes that the reader of this report is already familiar with the contents of the first review report. Text from that report is not repeated here unless it is directly relevant to addressing the specific issues noted above.

1.3. Documentation reviewed

SKB's principal description of the approach to safety assessment is in the Main Report (TR-14-01). This is supplemented by a series of supporting reports describing the initial state of the disposal system, the processes that will affect the evolution of the system, and the models and supporting data that have been used to calculate the consequences of system evolution in terms of doses to members of the public and to non-human biota.

This review is based on information provided in the Main Report, the Initial State Report (TR-14-02), the FEP Report (TR-14-07), and the Handling of Future Human Actions Report (TR-14-08). Extensive reference has also been made to specific parts of the Process Reports (TR-14-03, TR-14-04 and TR-14-05), the Radionuclide Transport Report (TR-14-09), and the Data Report (TR-14-10) and to selected SR-PSU supporting references.

2. FEP Handling

2.1. Introduction

The main issue addressed in this section is as follows:

- A detailed review of the reference evolution and the derivation of the main scenario could build confidence in the appropriateness of the assumptions made. This could include a check that all the FEPs identified in Step 1 of SKB's assessment methodology as being likely to occur are accounted for in the appropriate models.

2.2. SKB's approach

SKB's approach to the handling of FEPs in the SR-PSU assessment comprises the compilation of an initial FEP catalogue, an audit of this catalogue against other FEP lists, designating FEPs as being relevant to the initial state of the disposal system or

[1] Note: topics 3 and 4 were each split into two issues by SSM, but in conducting and reporting this review it was found most convenient to deal with the two issues together as they are closely related in both cases.

to internal or external processes acting on the disposal system, and allocating FEPs to particular components of the disposal system. These steps lead to the establishment of the SR-PSU FEP catalogue, which comprises FEPs categorised as:

- Initial state FEPs.
- Processes in the system components waste form, packaging, BMA barriers, BTF barriers, silo barriers, BLA and BRT barriers, plugs and other closure components and the geosphere.
- Variables in the system components waste form, packaging, BMA barriers, BTF barriers, silo barriers, BLA and BRT barriers, plugs and other closure components and the geosphere.
- Biosphere FEPs, comprising biosphere processes, sub-systems and variables.
- External FEPs.

The expected initial state, long-term processes and a reference external evolution derived from the SR-PSU FEP catalogue are used to define the reference evolution for the repository system. Other external FEPs are used in the selection of scenarios.

The differentiation between variables and processes in the FEP catalogue has enabled the generation of influence and process diagrams that have in turn been used to ensure that the Process Reports describe all of the key processes and interactions. Interaction matrices showing the couplings between variables and processes have also been prepared.

2.3. Comments

Comments on SKB's overall approach to FEP management and scenario development are provided in [1]. Here, the consistency and traceability of SKB's FEP documentation has been checked, considering a number of FEPs selected from the FEP database – see Table 1. The information presented in the database and in the referenced documents has been checked to ascertain whether FEPs that are included in the safety assessment calculations have been appropriately described, and whether there is appropriate justification for FEPs that have been excluded. The more detailed review of gas formation and transport presented in Section 3, however, shows that the summary information may not clearly document the treatment of a FEP.

In general, there is an appropriate level of information included in the FEP database to support the treatment of the FEP in the SR-PSU assessment and, where required, the supporting references provide further information. As noted previously in [1], there is not always a clear distinction made for FEPs that have negligible influence: in places the same FEP may be described as "addressed", because the effects are included within those of a more significant FEP or separate scoping calculations have been made outside the SR-PSU assessment, or "neglected". The review of gas formation and transport presented in Section 3 highlights this issue.

Table 1 Cross check of a random selection of FEPs to their treatment in SR-PSU.

Section	Process	FEP Name	Principal report reference in FEP database	Report sections referenced in database	Comments
Waste form	WM02	Radiation attenuation/heat generation	TR-14-03	3.1.2, 5.1	FEP not accounted for in SR-PSU, justification provided
Waste form	WM03	Radiolytic decomposition of organic material	TR-14-03	3.1.3, 5.1	FEP “accounted for” in SR-PSU through gas generation model but arguments presented that all aspects of FEP are negligible and FEP is not explicitly treated
Waste form	WM06	Phase changes/freezing	TR-14-03	3.2.2, 5.1	FEP accounted for in SR-PSU by choice of parameter values
Waste form	WM08	Water transport under saturated conditions	TR-14-03	3.3.2, 5.1	FEP accounted for in SR-PSU through numerical modelling
Waste form	WM10	Advective transport of dissolved species	TR-14-03	3.5.1, 5.1	FEP accounted for in SR-PSU
Waste form	WM15	Degradation of organic materials	TR-14-03	3.5.6, 5.1	FEP accounted for in SR-PSU through rates of cellulose degradation
Waste form	WM22	Transport of radionuclides in the gas phase	TR-14-03	3.6.3, 5.1	FEP not accounted for in SR-PSU through argument that methane production is negligible
Waste packaging	Pa05	Fracturing/deformation	TR-14-03	4.3.1, 5.1	Application to concrete included under WM09 Not accounted for in relation to steel packaging - no requirements
Waste packaging	Pa07	Diffusive transport of dissolved species	TR-14-03	4.4.2, 5.2	Application to concrete included under WM11 Not accounted for in relation to steel packaging - justification provided
Waste packaging	Pa10	Dissolution, precipitation and recrystallisation	TR-14-03	4.4.5, 5.2	FEP accounted for in SR-PSU through degradation rate of concrete

Section	Process	FEP Name	Principal report reference in FEP database	Report sections referenced in database	Comments
Waste packaging	Pa13	Gas formation and transport	TR-14-03	4.4.8, 5.2	FEP accounted for in SR-PSU through production of hydrogen, but no delay or damage assumed
Waste packaging	Pa15	Transport of radionuclides in the water phase	TR-14-03	4.5.2, 5.2	FEP accounted for in SR-PSU
1-2BMA	BMABa01	Heat transport	TR-14-04	5.1.1	Repository temperature treated as boundary condition Heat transfer not explicitly accounted for in SR-PSU - justification provided
1-2BMA	BMABa03	Water uptake and transport during unsaturated conditions	TR-14-04	5.2.1	FEP accounted for in SR-PSU though calculation of time to saturation
1-2BMA	BMABa06	Mechanical processes	TR-14-04	5.3.1	Aspects of FEP accounted for in SR-PSU Justification provided for neglected aspects
1-2BMA	BMABa11	Colloid stability, transport and filtering	TR-14-04	5.4.5	FEP not accounted for in SR-PSU - justification provided
1-2BMA	BMABa18	Transport of radionuclides in the water phase	TR-14-04	6.5.3	FEP accounted for in SR-PSU - description provided in Section 6.5.2 not 6.5.3
1-2BTF	BTFBa06	Mechanical processes	TR-14-04	6.3.1	Aspects of FEP accounted for in SR-PSU Justification provided for neglected aspects
1-2BTF	BTFBa15	Gas formation	TR-14-04	6.4.9	FEP accounted for in SR-PSU through analysis of gas build-up and redox conditions
Silo	SiBa02	Phase changes/freezing	TR-14-04	7.1.2	FEP accounted for in SR-PSU - applicability to concrete discussed in Section 5.1.2
Silo	SiBa04	Water transport under saturated conditions	TR-14-04	7.2.2	FEP accounted for in SR-PSU
Silo	SiBa08	Advection and dispersion	TR-14-04	7.4.1	FEP accounted for in SR-PSU (excluded for functioning bentonite barriers)
Silo	SiBa16	Osmosis	TR-14-04	7.4.9	FEP “accounted for” in SR-PSU but arguments presented that FEP is negligible and FEP is not explicitly treated

Section	Process	FEP Name	Principal report reference in FEP database	Report sections referenced in database	Comments
1-5BLA	BLABa09	Sorption	TR-14-04	8.4.3	FEP accounted for after saturation, neglected prior to this - justification provided
1-5BLA	BLABa16	Transport of radionuclides in the gas phase	TR-14-04	8.5.3	FEP treated through separate simplified case - justification cross-references to BMABa19 (see detailed comments in Section 3)
BRT	BRTBa03	Water uptake and transport during unsaturated conditions	TR-14-04	9.2.1	FEP not explicitly accounted for in SR-PSU - justification provided
BRT	BRTBa12	Aqueous speciation and reactions	TR-14-04	9.4.6	FEP accounted for in SR-PSU
BRT	BRTBa13	Microbial processes	TR-14-04	9.4.7	FEP not accounted for in SR-PSU, justification provided, but assumption identified as major uncertainty (see detailed comments in Section 3)
BRT	BRTBa17	Transport of radionuclides in the water phase	TR-14-04	9.5.1	FEP accounted for in SR-PSU
Plugs	Pg06	Piping/erosion	TR-14-04	10.2.4	FEP accounted for in SR-PSU through analysis of mass loss of bentonite
Plugs	Pg16	Montmorillonite colloid release	TR-14-04	10.4.9	FEP not explicitly accounted for in SR-PSU - justification provided
Plugs	Pg20	Transport of radionuclides in the water phase	TR-14-04	10.5.2	FEP not explicitly accounted for in SR-PSU but handled indirectly through hydrological model
Geosphere	Ge03	Groundwater flow	TR-14-05	3.1, 7.1	FEP accounted for in SR-PSU
Biosphere	Bio01	Bioturbation	R-13-43, R-14-02	6.1.1, 2.4.1	FEP accounted for in radionuclide transport model through selection of parameter values
Biosphere	Bio13	Primary production	R-13-43, R-14-02	6.1.13, 2.4.12	FEP accounted for in SR-PSU
Biosphere	Bio28	Water supply	R-13-43, R-14-02	6.3.9, 2.4.25	FEP accounted for in SR-PSU
Biosphere	Bio42	Exposure	R-13-43, R-14-02	6.5.2, 2.4.39	FEP accounted for in SR-PSU

2.4. Summary

The FEP Report and associated FEP database have been reviewed through a series of spot-checks. These demonstrate that SKB has taken a methodical approach to establishing the relationships between FEPs from a number of sources.

In addition to a list of FEPs, the FEP database also provides a summary description of how each FEP is handled in SR-PSU. Because of the several different disposal concepts within the SFR, there are separate descriptions for the scope and treatment of internal processes for each of the vault types as well as for the waste form and the packaging. This approach, rather than a single description covering all components of the engineered barrier system (EBS), helps to improve transparency in the treatment of FEPs.

The summary descriptions in the FEP database are not always sufficient to fully understand how a FEP has been treated. Cross-referencing to supporting reports generally provides further details, although a detailed review of some FEPs shows that these descriptions are not always adequate.

The significance of many FEPs in terms of post-closure performance is small. Such FEPs can reasonably be excluded from models, particularly where the uncertainty associated with other, more significant FEPs is large. SKB's terminology regarding these excluded FEPs is not always clear. Some are categorised as "neglected", whereas others are "addressed" even where there is no explicit treatment described. A more consistent terminology must be applied if the treatment of FEPs throughout the assessment is to be understood.

3. Gas formation and transport

3.1. Introduction

The main issue addressed in this section is as follows:

- The assumptions and modelling treatment of gas formation and transport, and its effects on groundwater flow and radionuclide transport in different parts of the repository. Have the methods for scenario selection been adequately described that were used for the identification of the most important course of events, given the FEP analysis and reference evolution?

3.2. SKB's approach

SKB considers the amount of gas that could be generated in the repository from (1) initial aerobic and then anaerobic corrosion of metals to generate hydrogen, (2) microbial degradation of organic wastes to produce a range of gases, and (3)

radiolysis (focusing on radiolytic decomposition of water to generate hydrogen and oxygen). SKB states that the third source is insignificant compared to the second source owing to the relatively low level of radioactivity in the waste.

SKB considers two aspects of the gas that is produced: the potential for pressure build-up within the repository and its implications, and the potential for transport of gaseous radionuclides such as C-14 in a gas phase.

3.2.1. Gas pressure build-up

Gas pressure build-up is of particular concern in the silo because the silo will be fully surrounded by bentonite and bentonite-sand mixtures. The function of the bentonite surrounding the silo is to limit water flow through the silo by providing a low permeability. However, the potential for gas pressure build-up is assessed for all vaults.

Gas formation rates are calculated as a function of time for structures, packaging, reinforcement in packaging, and waste. SKB considers the possibility that gas formed inside the silo and inside other vaults will create an over-pressure and expel contaminated water. This could occur as early as a few years after closure, when corrosion of aluminium in the waste will dominate gas formation, although dissolved concentrations of radionuclides will still be relatively low at such early times. SKB conservatively assumes instant dissolution of radionuclides when chemical conditions allow, with concentrations determined by a K_d approach. These modelling assumptions maximise the calculated gas generation rates at specific times.

SKB calculates gas generation rates, volumes and pressures in [2] and [3]. In the assessment calculations, however, gas generation by microbial degradation is excluded during the period where there is a high pH in the vaults (effectively the full assessment timescale of 100,000 years), because microbial activity is assessed to be limited at pH > 12.6.

Just considering the silo, in the main scenario, SKB assumes that gas vents ("evacuation pipes") built into the silo structure function as intended, so that there is no gas pressure build-up. An alternative assumption is that the vents do not fulfil their safety function. As gas pressure builds up in the silo, the gas will preferentially follow paths at interfaces between bentonite and other materials, and is likely to propagate to the base of the silo where it will escape through the bentonite-sand mixture. SKB states that the consequences of postulated gas pressure build-up have been evaluated to be small for the silo (and for other vaults) [2], so SKB does not identify a scenario to evaluate the effects of a gas pathway being established.

3.2.2. Release and transport of gaseous radionuclides

Displacement of vault pore water containing radionuclides is modelled as a function of gas formation in the vaults (FEP WM19). However, the transport of radionuclides in a gas phase has not been considered directly in the assessment calculations; rather, this issue is said to be treated via "scoping calculations" (FEP WM22) or via a "separate simplified case" (vault-specific FEPs concerning internal processes).

The generation of a gas phase can facilitate transport of gaseous radionuclides. The key gaseous radionuclide of concern is said to be C-14. The activity of microbes under anaerobic conditions may lead to significant production of gases such as CH_4, CO_2, and H_2. C-14 can be released as radioactive CH_4 and CO_2. However, owing to carbonation of the cement present in the near field, bulk CO_2 is assumed to be removed and radioactive CO_2, generated largely by degradation of C-14 labelled organic compounds within the waste, is assumed to be immobilised. This reaction is also assumed to limit the formation of radioactive CH_4 by methanogenesis.

In Appendix I of the Main Report, SKB notes requirements on pH control and the amount of cellulose in the repository. The presence of hyperalkaline water in the repository owing to the presence of cementitious materials is assumed to limit methanogenesis, but SKB notes that further research is required and that pH in the vaults where C-14 is abundant is required to be above 12.5 until a substantial portion of the C-14 has decayed.

The geosphere is assumed to provide no delay in the release of gases generated in the repository into the biosphere.

3.3. Comments

3.3.1. Gas pressure build-up

Gas pressure build-up in the repository has been assessed by SKB and is said to be of insignificant concern. The documentation should be improved because *gas pressure* is identified as a key safety function indicator for the silo. If the consequence of not meeting this safety function are thought to be unimportant, why does it remain as an important safety function indicator?

The rationale for considering gas pressure build-up to be unimportant is not contained in the safety case itself, but is referenced out to [2]. Ideally the logic for including or excluding particular scenarios would be presented in the safety case Main Report or one of the principal supporting reports.

The referenced report considers the implications of a relatively small quantity of water contaminated by radioactivity being expelled from the vaults owing to relatively rapid gas pressure build-up (first 2.5 years after closure). At these short timescales, the pore water in the vaults still contains relatively low concentrations of radionuclides and the total pore space is generally limited in most vaults, so it is not surprising that the consequence of releasing this quantity of contaminated water is relatively insignificant. However, the assessment reported in [2] does not consider the potential impacts of release of gaseous radionuclides.

Microbial degradation as a source of gas generation is discounted because it is assumed that the pH will remain above 12.6 for the full assessment timescale of 100,000 years. Notwithstanding the fact that some of the vaults do not contain any cement conditioning (e.g. BLA vaults), it is not clear where SKB demonstrates that there is sufficient cementitious material in each vault to provide adequate cement conditioning over this timescale. The longevity of the cement will relate in part to groundwater flow and rates of cement dissolution and erosion.

In terms of scenario development, therefore, the treatment of gas pressurisation should be further clarified and justified by SKB.

3.3.2. Release and transport of gaseous radionuclides

When SKB refers to gas transport being considered via a separate calculation, it is unclear what calculation they are specifically referring to. As an example of the confusion, the Engineered Barrier Process Report notes that for the 1BMA vaults, "Since the prediction of gas generation over time is difficult, the gas accumulation and release calculations are studied for different scenarios" (page 65). It also states that "For calculation cases where significant amounts of radionuclides are assumed to be released in the gase (sic) phase, the whole release is assumed to reach the surface system (Biosphere) directly, i.e. at the same rate as gas is generated in the repository" (page 145). Similar statements are made for the Silo (e.g. page 188). However, as noted above, there are in fact no scenarios in SR-PSU that explicitly investigate gas phase releases.

There is also poor traceability in terms of statements made about the handling of uncertainty in SR-PSU concerning transport of radionuclides in the gas phase. For example, in the Engineered Barrier Process Report, in the sections on handling of uncertainty the reader is cross referred to a discussion of the handling of uncertainty concerning transport of radionuclides in the water phase, which is not at all relevant. The Waste Form and Packaging Process Report (Section 3.6.3) notes that "…the release of C-14 as methane is handled by approximate calculations", but it is again not clear what calculations are being referred to.

The main source of scoping calculations appears to be SR-PSU supporting references [2] and [3]. However, neither of these reports actually calculates doses, and they mainly update selected calculations from earlier reports. A much earlier (2001) report [4] does present scoping calculations and safety arguments pertaining to release of gaseous radionuclides, but these calculations are limited to the first 1,000 years after closure. On these timescales, the repository is still below the Baltic Sea, and the report concludes that potential releases to the biosphere of H-3 and C-14 could be significant, but would be massively diluted. No consideration is given to other potential gas phase releases, e.g. Rn-222, in these reports.

The later report [3] assesses the potential implications of release of C-14 (only) in the form of methane on longer timescales, but does not go so far as to illustrate safety implications. It concludes that it is critical to control conditions in the repository to avoid releases of C-14. SR-PSU is based on the assumption that releases of C-14 in the gas phase will be suitably controlled, so that this is not considered in the main scenario or in any alternative scenarios. Overall, it seems like an oversight in the assessment that such a potentially important issue, where SKB acknowledges uncertainty and suggests the need for further research and development of waste acceptance criteria (WAC), does not form part of a scenario or at least a sensitivity study.

There is no equivalent discussion of the potential for transport of other radioactive gases, including gases that arise as decay products owing to disposal of parent radionuclides (e.g. Rn-222). However, SKB acknowledges that free gas able to enter the host rock could be transported rapidly to the surface environment, so that

even gaseous radionuclides with relatively short half-lives could have a radiological impact. The Geosphere Process Report (Section 6.3.7) indicates that the release of both C-14 and Rn-222 from the repository to a point directly above the repository should be assessed in SR-PSU, but this does not appear to have been done. This report also notes that there is considerable uncertainty concerning the form of any C-14 that would be released, and the potential for Rn-222 to decay significantly (because of its relatively short half-life) before it reaches the biosphere (as noted above, transport through the geosphere in a gas phase is conservatively assumed to be instantaneous).

SKB notes the following key assumptions regarding internal processes or evolution of the repository system (SR-PSU Main Report, Section 11.5.1):

1. The load exerted by swelling waste will not damage the barriers in 1BMA and 2BMA.
2. The quantity of reactive metals is so low that the barriers are not damaged by gas.
3. The pH 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.
4. The quantity of cellulose in the waste is limited, to avoid concentrations of the complexing agent isosaccharinate (ISA) that could adversely affect the sorption of radionuclides.

Assumptions 2 and 3 directly concern the potential for gas pressurisation and transport of gaseous radionuclides, and need to be considered in the WAC. The quantity of cellulose is also important with regard to gas generation potential (although here SKB only cites its importance for ISA).

The BLA vaults do not contain any cementitious conditioning in the waste packages or any backfill, so voidage is extremely high. There may not be a significant availability of C-14 in the wastes or potential for other gaseous radionuclides to arise in these vaults. However, to the extent that they do, arguments made for the vaults containing cementitious materials are not appropriate as there will be no conditioning to high pH (the vault chemistry will be near neutral).

3.4. Summary

Gas pressure build-up in the repository has been assessed by SKB and found to be of insignificant concern. However, this is based on an assumption in the safety assessment calculations that only corrosion of metals contributes to gas formation. In fact, there is significant uncertainty on how much gas might be generated by microbial degradation of organics, and the total volume could be a significant fraction of that generated by corrosion (reference SKB's own calculations in [2] and [3]).

One important uncertainty pertains to whether methanogenesis could be active at high pH, which is identified by SKB, who call for further research on this topic. Given the uncertainties, it would be appropriate to consider a scenario, or at least sensitivity studies, in which methanogenesis is active, and therefore there is a potential for release of C-14 from the repository in a gas phase.

Clearer and more consistent explanation is needed of why other gaseous radionuclides are not considered in assessment calculations.

4. Risk summation and risk dilution

4.1. Introduction

The main issues addressed in this section are as follows:

- Is SKB's method for risk summation appropriate?
- Has risk dilution handled in an appropriate manner?

4.2. SKB's approach

4.2.1. Risk summation

Risk has been calculated based on a probabilistic analysis of parameter value uncertainty for individual scenarios to derive mean doses for these scenarios. A maximum probability for the less likely scenarios have been calculated (generally 0.05 or 0.1) and the peak mean annual dose has been multiplied by this probability to determine an annual "risk" for each scenario. The probability of the main scenario is conservatively assumed to be 1. These calculated risks have then been summed to determine an overall peak risk. The general approach to risk evaluation can be summarised as follows:

1. Calculate the conditional risk, i.e. based on the mean dose for each calculation case.
2. Weight the results from the different calculation cases by their probabilities of occurrence to obtain a total risk estimate as a function of time.
3. Compare the estimated time-dependent risk with the risk criteria in the regulations.

Several combinations of two scenarios are evaluated by SKB, but excluded from the risk summation owing to an assumed low likelihood and moderate calculated dose, resulting in small contributions to total risk.

All less probable scenarios, except human intrusion scenarios, are considered to be mutually exclusive with respect to the main scenario, i.e. either the main scenario or a less probable scenario can occur, but not both, so the risks of these less probable scenarios cannot be added to the risk of the main scenario. The combined radiological risk of the main scenario and the mutually exclusive less probable scenarios is calculated as the sum of the main and the less probable scenarios, weighted by their respective probabilities. On the other hand, the total risk of the main scenario and the well scenarios is calculated by assuming a probability of 1 for the main scenario and adding the risk of the well scenarios.

4.2.2. Risk dilution

SKB limits its consideration of risk dilution to *"...situations where a probabilistic approach tends to spread an exposure that will occur at a certain point in time over several future generations, since the time of occurrence is uncertain*" (SR-PSU Main Report, Section 2.3.2). SKB considers that probabilistic calculations can in certain cases give an insufficient picture of how an individual detrimental event would affect the risk for a particular generation. In light of this, SKB has taken a different approach to calculating risk for the earthquake scenario and the well scenarios. Calculations of the risk associated with these scenarios have been made by summing the risk from individual simulations (i.e. they are not averaged as for other scenarios).

SKB does not discuss the issue of risk dilution with regard to the probabilistic calculations of dose and risk for any other scenario.

4.3. Comments

4.3.1. Risk summation

The approach used by SKB to risk summation contains a number of conservatisms and is appropriate for determining a value of annual risk to compare with regulatory guidance (generally 10^{-6}, or 10^{-5} where only a few people are expected to receive the exposure).

However, this approach cannot be used to consider approaches to optimise the design and determine a suitable inventory for particular vaults. As discussed in [1], optimisation has not been considered directly in the safety case, although it is identified as a forward action as part of an iterative cycle of safety and design assessment (Chapter 11 of SR-PSU Main Report).

All scenarios except the direct intrusion scenarios meet or just exceed the regulatory risk criteria even without considering the probability of the scenario. The next most important scenario in terms of calculated mean dose is the *high inventory scenario*, and then the scenario with wells downstream from the repository and the earthquake scenario. Therefore, it is particularly important to consider the assessed probability of occurrence of these scenarios. The assessed probabilities are 2 to 8 x 10^{-4} for *intrusion wells* into different vaults, <0.05 for the *high inventory scenario*, 0.13 for the *wells downstream from the repository* into a radionuclide plume, and 10^{-6} per year for the *earthquake scenario*.

First, as noted in [1], it is unclear why SKB has included *intrusion wells into the repository* as a separate less probable scenario rather than as part of the residual scenario assessing future human actions, which also considers the impacts of intrusion wells into the repository. Drilling into the vaults has the potential to give rise to conditional risks several orders of magnitude greater than the regulatory risk criteria.

In the *high inventory scenario*, the inventory of a radionuclide is set to the 95th percentile of its activity distribution. This scenario is then assigned a probability of

occurrence of <0.05. However, as noted in [1], it seems inappropriate to derive a less probable scenario with an arbitrary increase in the overall inventory. Investigation of the effects of an increased inventory would be better implemented through the calculation of specific doses (i.e., the dose arising from a unit disposal activity). By calculating these for each vault type and each radionuclide, the effects of varying waste volumes, waste stream compositions, and of consigning wastes to different vaults could be readily assessed. The sum of fractions approach could then be used to monitor disposals as they occur and ensure that the overall radiological capacity of the repository is not exceeded.

With regard to *wells downstream from the repository*, SKB derives a probability of occurrence for this well by estimating the current areal distribution of wells in the Forsmark area (0.5 wells per km^2) and multiplying this by a well interaction area (an area where there is a high density of groundwater flow pathways from the repository in the depth range 10-80 m below present-day sea level = 0.26 km^2). However, this calculation seems arbitrary as the pattern / frequency of drilling may be substantially different in the future, particularly as land uplift continues. In fact, a well downstream from the repository is likely to occur at some point over the assessment timescale. This calculation is important because, aside from the main scenario (calculated peak annual risk = 4×10^{-7}), this scenario has the greatest calculated risk (1.4×10^{-7}). This is discussed further below (risk dilution).

4.3.2. Risk dilution

The approach to considering risk dilution for the earthquake and well scenarios is appropriate, albeit this review has questioned the overall presentation of the direct intrusion well scenario. The impact of considering risk dilution in the manner described by SKB is to increase the calculated risk for the scenario *intrusion wells into the repository* by up to several orders of magnitude, such that the peak annual risk is just below the upper value of the regulatory risk criteria (10^{-5}). The peak annual risk for the scenario *wells downstream from the repository* increases so that it just exceeds the lower value of the regulatory risk criteria (10^{-6}).

As noted above, there is no discussion by SKB of the possibility of risk dilution for other scenarios, linked with the conduct of probabilistic calculations considering parameter value uncertainty. It is possible that there are situations where an overly broad consideration of uncertainty in a particular parameter value could give rise to risk dilution, but this issue is not examined by SKB.

SKB acknowledges the importance of supplementing probabilistic calculations by deterministic calculations. The mean calculated annual dose from probabilistic calculations is compared to the best estimate value in a deterministic calculation, and the former is shown to be greater. Various percentiles from the probabilistic calculations are also presented (along with the median values). However, other than a best estimate calculation case, there is no presentation of particular deterministic calculations in the radionuclide transport calculations to explore the potential importance of particular simulations, or to examine parameter value combinations that might give rise to the largest calculated risks.

4.4. Summary

SKB's approach to risk summation is conservative, and is well suited to comparison against regulatory performance measures. However, it not possible to use such an approach for optimisation studies.

Risk dilution is considered by SKB with regard to the earthquake and well scenarios, but its potential importance is not explicitly considered with regard to the treatment of parameter value uncertainty in the probabilistic calculations for other scenarios.

5. Treatment of uncertainties in initial state of the barriers and identification of design basis cases

5.1. Introduction

The main issues addressed in this section are as follows:

- Has the treatment of uncertainties in the initial state of the barriers and possible malfunctions been adequately described*?*
- Have a number of design basis cases been adequately identified based on scenarios that can be shown to be especially important from the standpoint of risk?

The question of design bases stems from the general advice to section 9 of SSMFS 2008:21:

> *A number of **design basis cases** should be identified based on scenarios that can be shown to be especially important from the standpoint of risk. Together with other information, such as regarding manufacturing method and controllability, these cases should be used to substantiate the design basis, such as requirements on barrier properties.*

5.2. SKB's approach

The initial state FEPs in the SR-PSU FEP catalogue are either related to an initial state in conformity to the specification given for the design or to deviations from the reference design. The FEPs that are related to deviations are shown in Table 2. ISGen02, ISGen03 and ISGen05 are included in the assessment either explicitly (03 and 05) or implicitly (02).

Table 2: Initial state FEPs related to deviations from the expected initial state and how they are handled in SR-PSU (Main Report, Table 3-1).

Safety principle	Breaks down into safety functions
ISGen01 Major mishaps/accidents/sabotage	Excluded. The probabilities for such events are low. If they occur, this will be known prior to repository sealing, so mitigation measures and assessments of possible effects on long-term safety can be based on the specific real event.
ISGen02 Effects of phased operation	Excluded from explicit consideration, as its implications are included in the definition of the initial state.
ISGen03 Incomplete closure	Considered in selection of scenarios.
ISGen04 Monitoring activities	Excluded. Monitoring activities that could disturb the repository safety function will not be accepted.
ISGen05 Design deviations - Mishaps	Covered by the data uncertainty ranges that are used.

Uncertainties in the initial state are considered with respect to the safety functions of each barrier, and are accounted for in the safety case by consideration of a parameter value distribution in the probabilistic calculations for the main scenario and/or as a basis for defining an alternative scenario, depending in part on the significance of the uncertainty as judged by SKB.

For example, the safety function *low flow in the bedrock* is assessed using two safety performance indicators: *hydraulic conductivity* and *hydraulic gradient*. Uncertainties in groundwater flow through the waste vaults are considered to be sufficiently significant that a less probable scenario is identified and modelled – the *high flow in the bedrock scenario*. The main scenario considers an intermediate flow rate through all waste vaults, considering a suite of 17 groundwater flow cases having different parameterisations of deformation zones and the fracture network. For the *high flow in the bedrock scenario*, hydrogeological data for a bedrock case (case 11) that represents high flow were used for the radionuclide transport calculations in the geosphere. Flow rates through each waste vault were conservatively scaled considering the full range of uncertainty in flow simulations.

In contrast, as noted above in Section 3, the potential effects of gas pressure build-up in the silo are assessed to be sufficiently small that no separate scenario is required.

Design bases are considered by SKB via development of scenarios that examine assumptions and uncertainties concerning the initial conditions of the design. As discussed in [1], the less probable scenarios are developed via a structured approach, and a further set of residual scenarios is identified to illustrate, in part, the significance of individual barriers and barrier functions regardless of probability. Overall, SKB indicates that uncertainties in the initial state are considered via three less probable scenarios and two residual scenarios (see Figure 2):

- High inventory (assessed probability less than 0.05)
- High concentrations of complexing agents (assessed probability less than 0.1)
- High flow in the bedrock (assessed probability less than 0.1)
- Changed repository redox conditions in SFR 1 (residual scenario)
- Unclosed repository (residual scenario)

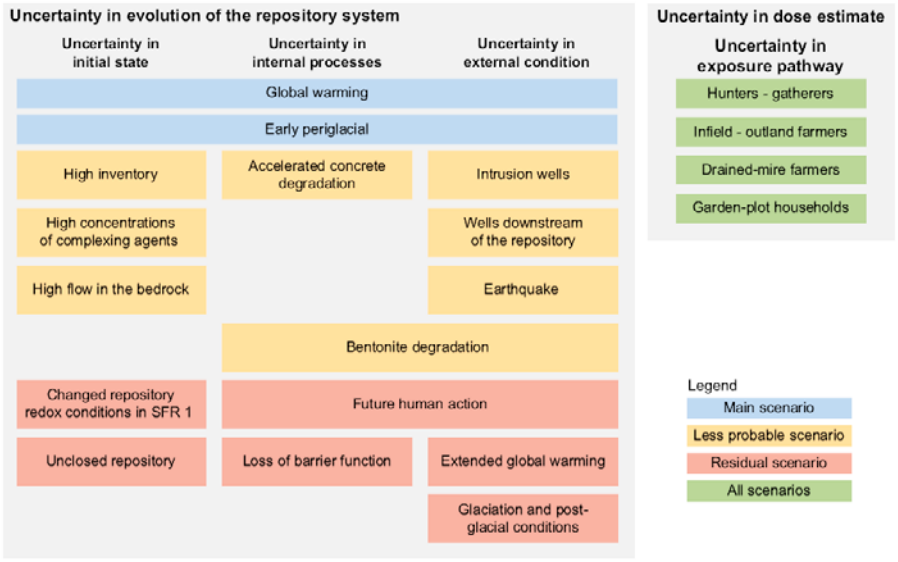

Figure 2 Illustration of how uncertainties are handled in the scenarios for the long-term safety assessment SR-PSU (Main Report, Figure 7-16).

5.3. Comments

Of the FEPs relating to deviations from the initial state (Table 2), we note the following:

- Known malfunctions (ISGen01) are excluded from consideration in the assessment, and this seems an appropriate assumption (especially where they are considered to be of low probability). It also seems appropriate to exclude monitoring activities (ISGen04) that would anyway not be permitted. Phased operation (ISGen02) is part of the operational management plan for the SFR, so does not actually represent a deviation from the initial state.
- Incomplete closure (ISGen03) is considered as a residual scenario by SKB (Figure 2), as required by SSM.
- Undetected mishaps (ISGen05) are considered in developing parameter value distributions for assessment modelling, but are not identified by SKB as scenario forming.

However, we note that some of the scenarios that have been established by SKB to examine uncertainties in internal processes (e.g. accelerated concrete degradation, bentonite degradation, loss of barrier function, Figure 2) also effectively examine initial state assumptions and uncertainties. For example, accelerated concrete degradation could arise from uncertainty in the processes that give rise to concrete degradation or larger than assumed uncertainties in the initial state of concrete structures. This scenario is not intended by SKB to examine initial state uncertainties, and SKB claims that such structures will not be subject to sufficiently large initial state uncertainties to require separate development of a less probable scenario. However, this scenario differs from the main scenario by assuming that the hydraulic conductivity of the concrete increases earlier or to a greater extent than in the main scenario (global warming calculation case). Therefore, it may also

provide some insight into the possible impacts of alternative assumptions concerning the initial state of the concrete in the vaults. Similarly, one of the *loss of barrier function calculation cases* assumes high water flows in the repository by applying near-field flows, porosities and diffusivities for completely degraded concrete and bentonite barriers.

SKB models all of the vaults as if they are independent of each other. The main discussion provided of the potential for interactions between vaults is through consideration of the need for plugs for particular vaults, but this is considered mainly in the context of radionuclide transport calculations. There is no consideration of potential thermal, hydrological, mechanical, chemical, gas and biological (THMCGB) interactions between the evolving vaults via the host rock. Overall, further discussion of the potential THMCGB interactions that considers both the access ways and the host rock is needed. For example, the BLA vaults do not contain any cementitious conditioning in the waste packages or any backfill, so voidage is extremely high. This will lead to gradual collapse of the vaults over time, with potential mechanical and hydrological effects on the near-field host rock. Could this have any implications for performance of neighbouring vaults? Similarly, could there be any chemical interactions between neighbouring vaults, e.g. vaults conditioned to high pH and those that have no conditioning (e.g. BLA vaults)?

SKB notes that it will be necessary to repair and reinforce the concrete structures within the 1BMA vault prior to closure (Initial State Report, Sections 4.3 and 4.4). However the closure plan is not published and was not available for review as part of the SR-PSU assessment. It is therefore unclear what the specific issues are that require optimisation measures, and what measures are proposed / planned. However, the fact that the 1BMA structures are considered to be insufficient in their current state means that there is still uncertainty on what their eventual state at the time of closure might be. The SR-PSU assessment appears to assume that some undescribed remediation will be put in place to ensure a particular "initial state" at the time of closure, albeit all of the design data provided relates to the current state of the vault. It would have been useful for the assessment to have included sensitivity studies specifically identifying current issues with the 1BMA structures and potential performance if the 1BMA structures were left as is, and the potential impacts on safety of possible remedial measures. Not least, an understanding of issues associated with the 1BMA structures would be valuable in terms of understanding and justifying design improvements in the proposed new vaults (in particular 2BMA, Section 5 of the Initial State Report).

5.4. Summary

Overall the approach to treating uncertainties in the initial state of the barriers is adequately described. Design basis cases have been identified based on a set of less probable and residual scenarios. The residual scenarios do not contribute to SKB's overall assessment of risk, but they do illustrate barrier significance.

SKB should assess the potential for THMCGB interactions between vaults.

SKB should conduct sensitivity studies to examine the need for optimisation of the 1BMA vaults.

6. Reasonableness of assumptions and calculated doses in FHA cases

6.1. Introduction

The main issue addressed in this section is as follows:

- The dose calculations in the FHA cases should be reviewed, including cases exposure of the on-site crew during the drilling event, exposure during construction on drilling detritus landfill, exposure due to cultivation on drilling detritus landfill, and the unclosed repository calculation case. The reasonableness of the assumptions made and the resulting doses should be assessed.

6.2. SKB's approach

SKB's consideration of future human actions that might affect the disposal system and the results of consequence calculations for human intrusion are presented in the Handling of Future Human Actions Report (TR-14-08). SKB has identified a range of societal and technical FHA FEPs and assessed the potential effects of these on the safety functions associated with components of the repository. This analysis identified the drilling of a well as the principal FHA scenario requiring quantitative assessment. Water management and underground construction were also identified as having potential consequences but further arguments were presented to show these consequences to be negligible.

For the drilling scenario, three calculation cases were defined to calculate the potential doses to members of the drilling crew and to members of the public exposed to contaminated material removed during drilling.

6.3. Comments

SKB's overall approach to the identification and analysis of FHA builds confidence in limiting the quantitative assessment to the drilling scenario. SKB's assumptions and parameter value choices relating to this assessment have been reviewed and discussed below in terms of:

1. Intrusion time.
2. Drilling techniques.
3. Exposure of the on-site crew during a drilling event.
4. Exposure during construction on drilling detritus landfill.
5. Exposure due to cultivation on drilling detritus landfill.
6. The unclosed repository calculation case.

6.3.1. Intrusion time

All of SKB's calculations of the potential consequences of FHA are based on the assumption that drilling through the repository would be unlikely to take place before 3000 AD. This is the time at which the site footprint is assumed to have emerged from the sea. This is a key assumption as radioactive decay in the period prior to this will significantly reduce the inventory and hence calculated doses. There is a possibility of drilling prior to emergence of the land, and the assumption of emergence at 3000 AD is based on a linear rate of land uplift that is subject to some uncertainties.

It would be informative for SKB to calculate the potential consequences of intrusion at times earlier than 3000 AD so as to demonstrate the significance of land emergence. If, for example, the consequences of drilling at 2300 AD were still consistent with the International Commission on Radiological Protection (ICRP) ranges of reference levels indicative of system robustness, i.e. a few mSv/y, this would provide further support to the case that FHA do not give rise to concern. Such a date would be consistent with the period of institutional control and retention of knowledge that is assumed by SKB for the repository for spent fuel.

6.3.2. Drilling techniques

SKB uses two sets of assumptions relating to the type of drilling undertaken: diamond core drilling with water and rotary drilling with air. These represent two of the seven drilling technique / drilling fluid combinations identified by [5] and other techniques are shown to result in higher doses (Figures 10 and 11 in [5]). An explanation of why these two techniques were selected should be provided.

SKB has limited its dose calculations to an assessment of drilling crews examining cores, although the description of the drilling techniques in Section 4.4.11 suggests that only the diamond core drilling with water technique would yield core. The assumption that the rotary drilling with air technique yields core rather than cuttings results in very large cores - a 1 m length core from the assumed size of borehole would weigh over 810 kg. Although drilling large diameter holes may be undertaken for specific engineering purposes, extracting cores of this size from depths over 120 m would be unusual. It would be more reasonable for the material extracted from such a borehole to be in the form of cuttings. This could affect the exposure pathways for members of the drilling crew in terms of different exposure times, distance from the source and dust loading.

The report from which SKB has derived its methodology for assessing doses from drilling [5] considers exposures to two groups: drilling workers and geological investigators. SKB, however, has only included exposures to the first of these without explaining why exposures to geological investigators have been omitted.

[5] presents what it terms "normalised doses", based on assuming an activity of 1 Bq/g of each radionuclide in the contaminated material hit by the drill, drilling into a 1 m length of contaminated material, and exposure for one hour. SKB has used these results to derive doses for intrusion into various parts of the repository based

on the inventory at different times. SKB has not, however, made any changes to the unit values for length of core or time of exposure. It is unclear whether SKB considers that exposure for 1 hour to a 1 m length of core represents realistic behaviour for a member of the drilling crew, or whether the reported doses are expected to be interpreted as unit exposures.

SKB makes the same assumption regarding a 1 m length of core for the exposure scenarios arising after drilling. If SKB does consider that such a short length of core is the only contaminated material that might be retrieved from drilling into the repository then a justification of this assumption is required. Otherwise, it would seem more reasonable to assume that material from the entire thickness of the repository was retrieved. This would apply particularly in the case of drilling without coring when it may be less obvious that the drill has penetrated man-made materials. In such a case, although the exposure of drilling crews might be reduced because cuttings are not examined as closely as core, the disposal of cuttings from the entire thickness of the waste would increase the exposure of groups working or cultivating contaminated land.

6.3.3. Exposure of the on-site crew during the drilling event

Members of the crew engaged in the drilling operation are assumed to receive a dose via three exposure pathways: external irradiation and the ingestion and inhalation of dust. SKB has reproduced the equations for calculating doses via these pathways from [5].

SKB has introduced a change in units for density in the equation for external exposure so this equation does not balance. The original equation in [5] has units of g/m^3 for density, whereas SKB uses kg/m^3 in the table of parameter values (Table 5-3 of the FHA Report). It is not clear from the results presented by SKB whether this difference has been propagated through to the calculated results. If it has, then the reported doses from this pathway would be three orders of magnitude lower than intended. As doses from other pathways are several orders of magnitude greater than those from external exposure, this potential error does not affect the overall doses reported.

In the equations describing the derivation of dose, SKB defines two variables (S_i and A_i) as the average activity concentration of a radionuclide in the sample. It would be clearer to use a single variable for this average activity. Alternatively, in the manner in which the equations are used, S_i could be defined as a unit activity (i.e., 1 Bq/g).

In Figure 5-2 of the FHA Report, SKB presents the contribution of different radionuclides to the total dose rate from different vaults. Although the different inventories would be expected to result in different sets of key radionuclides, there appear to be other selection criteria. For example, the calculated dose rate for Pu-242 would be about 7×10^{-9} Sv/yr at 3000 AD for the Silo, comparable to the dose from other radionuclides, but Pu-242 does not appear on the plot for the Silo (Figure 5-2a, FHA Report). The criteria used to select radionuclides for display should be made clear.

6.3.4. Exposure during construction on drilling detritus landfill

For this calculation case, SKB acknowledges that material brought to the surface from drilling would likely be in the form of detritus or cuttings as discussed above. This material is assumed to be disposed of in a small landfill that is then re-used as a construction site. SKB makes the same assumption as for the drilling crew - that only 1 m of waste is penetrated by the borehole. In practice, particularly when cuttings rather than core are brought to the surface, it is more likely that drilling would penetrate more waste packages and, hence, more contaminated material would be disposed of and then re-used.

SKB bases its assessment of doses during construction on [6]. This study considered four different patterns of contamination from which SKB has selected only one. This "exposed, uniform" pattern does give rise to the highest calculated doses, but SKB does not justify its selection in preference to the other, potentially more realistic, patterns.

[6] assumes construction workers would be on site and potentially exposed to contaminated material for 2,000 hours per year. SKB has reduced the site occupation time to 200 hours per year, with the justification that the amount of material from 1 m of borehole would only contaminate a small area. Further support is needed for this limited exposure time.

The assessment in [6] does not consider all of the radionuclides identified by SKB as relevant to the SR-PSU assessment, and SKB states that analogue dose conversion factors (DCFs) were used for the missing radionuclides. It would be useful to identify which of the DCFs were derived in this way and what basis was used to identify the analogues.

6.3.5. Exposure due to cultivation on drilling detritus landfill

This case is based on the same assumptions regarding the quantity of waste extracted during drilling and the same comments as made above apply.

SKB's assessment of doses for this case is based on the same biosphere model as used for other parts of SR-PSU and this model and its parameterisation have not been reviewed here. SKB assumes that a family lives on the contaminated site and consumes vegetables grown there over a 50-year life-time. By using average soil concentrations over this 50-year period, however, SKB reduces the overall calculated dose (Appendix C of the FHA Report). Because the earliest intrusion is at 3000 AD, radionuclides with a half-life shorter than 100 years will have largely decayed prior to intrusion and so this average concentration may not differ significantly from the concentrations at the time of intrusion. In-growth for some radionuclide chains may in fact increase concentrations over the 50-year period, but

SKB needs to justify that, overall, maximum dose rates are not being significantly under-estimated by this use of average concentrations.

SKB only presents doses to adults arising from the cultivation of contaminated ground. Higher DCFs and different consumption patterns may mean that infants and children would receive higher annual doses than adults. The use of life-time average concentrations as noted above is not a reason for not calculating doses to other age groups and SKB should justify its approach.

6.3.6. Unclosed repository calculation case

SSM's guidance (SSM 2008:21) requires SKB to assess the consequences of an unclosed repository, treating this as a residual scenario with no consideration of its probability of occurrence. SKB argues, without any further analysis, that it would take a long time to transport dissolved radionuclides from an unclosed repository to the Baltic Sea. Conversely, SKB also postulates that fresh-water could percolate into an unclosed repository and replace the saline water. Although apparently contradictory, the net result of these assumptions is the conservative assumption that a future population could drink water directly from the repository entrance.

The Radionuclide Transport Report (TR-14-09) notes that the unclosed repository scenario has been assessed deterministically using a simplified stirred tank model. No other references to the details of this approach or the nature of the simplifications from the stirred tank models used for other calculation cases have been found in the reports reviewed.

For the purposes of the unclosed repository calculation case, SKB considers both the anticipated inventory for the SFR and an additional inventory including wastes in interim storage awaiting disposal in the SFL. It is unclear what conclusions SKB consider can be drawn from the results for the latter inventory.

6.4. Summary

Overall, SKB uses its calculations of FHA to show that the potential consequences of drilling into the repository are consistent with the ICRP's ranges of reference levels indicative of system robustness. This conclusion is based on the earliest time of intrusion being 3000 AD, and on only 1 m of core or associated cuttings being extracted from the repository. These assumptions are subject to significant uncertainties and further calculations to support SKB's conclusions are required.

7. References

[1] R.D. Wilmot, 2015. Review of Safety Analysis Methodology in SKB's Safety Assessment SR-PSU: Initial Review Phase. In: SSM's external experts' reviews of SKB's safety assessment SR-PSU – radionuclide transport, dose assessment, and safety analysis methodology: Initial review phase. SSM Report 2016:09.

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[6] W.B. Oatway and S.F. Mobbs, 2003. Methodology for estimating the doses to members of the public from the future use of land previously contaminated with radioactivity. NRPB-W36, National Radiological Protection Board, UK.

APPENDIX 1

Coverage of SKB reports

The reports that have been covered in this review are listed in table A1.

Table A1-1: Reports that have been covered in this review.

Reviewed report	Reviewed sections	Comments
TR-14-01 Main report	All	
TR-14-02 Initial state report	All	
TR-14-03 Waste form and packaging process report	3.5, 3.6, 4.4, 4.5	
TR-14-04 Engineered barrier process report	1-2BMA: 5.2.3, 5.4.8, 5.4.9, 5.4.10, 5.5.3, and related sub-sections for other vaults	
TR-14-05 Geosphere process report	3.3, 6.3	
TR-14-07 FEP Report	All	
TR-14-08 Handling of future human actions	All	
TR-14-09 Radionuclide transport and dose calculations	All	
TR-14-10 and TR-14-12 Data report and Input data report		High level assessment of selected parts
Supporting reports as per list of references		To better understand summary statements concerning gas generation in SR-PSU safety assessment reports

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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.

The Authority reports to the Ministry of the Environment and has around 300 employees with competencies in the fields of engineering, natural and behavioural sciences, law, economics and communications. We have received quality, environmental and working environment certification.

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Arkitektkopia AB, Bromma, 2017