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Authors: Richard Little
Philip Maul
Peter Robinson
Claire Watson

Technical Note

2012:55

Review of SKB's Radionuclide Transport Methodology

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SSM perspektiv

Bakgrund

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

Projektets syfte

Syftet med detta granskningsuppdrag är att överväga om SKB: s metod för att sammanfatta FEP (egenskaper, händelser, processer) och platsspecifik information samt andra data i bedömningsmodeller för radionuklidtransport är lämplig och tillräcklig för sitt ändamål. Särskilt ska man undersöka om SKB: s tekniska argument är välgrundade, relevanta och tillräckliga för att ge stöd åt resultat och slutsatser.

Författarnas/Författarens sammanfattning

Som en del av SSM: s inledande granskningsfas av SKB: s SR-Site säkerhetsbedömning av slutförvaring av använt kärnbränsle i Forsmark har SSM gett Quintessa i uppdrag att överväga om SKB:s metod för att sammanfatta FEP (egenskaper, händelser, processer), samt plats- och andra data i bedömningsmodeller för radionuklidtransport är lämplig och tillräcklig för sitt ändamål. Denna Technical Note sammanfattar resultaten av Quintessa:s granskning.

Granskarna anser att SKB: s metodik förefaller vara lämplig och tillräcklig, men de konstaterar att det finns utrymme för förbättringar avseende tydligheten i dokumentationen. Information som är relevant för radionuklidtransportmetoden är utspridd i olika rapporter i stället för att sammanfattas i en enda rapport på hög nivå med referenser till detaljerade stödjande rapporter. Transparens och spårbarhet i rapporterna hindras av att det sällan finns avsnittsnummer vid hänvisning till andra SR-Site rapporter samt av det dominerande inslaget av probabilistiska beräkningar. Detta gör det mycket svårare för läsaren att få en god förståelse för vad som verkligen är viktigt (genomsnitt över ett stort antal realiseringar döljer viktiga inslag i beräkningarna) och hindrar reproduktion av SKB: s beräkningar av en tredje part.

Fullständigheten, den vetenskapliga grunden och kvaliteten av arbetet som granskades anses vara allmänt bra. Granskarna välkomnar särskilt användningen av analytiska och förenklade modeller för att komplettera användningen av numeriska modeller. Granskningen identifierade dock:

- begränsad information om vissa aspekter av metodiken t.ex. processen för utveckling av konceptuella modeller med FEP och platsspecifik information,
- begränsad motivering för införande/uteslutande av FEP i de granskade rapporterna;
- vissa luckor i de beaktade beräkningsfallen;
- vissa kvalitetssäkringsfrågor kopplade till data och beräkningar, samt
- frågor om lämpligheten hos gasberäkningar.

Gransknings- och analysbehov av SSM och dess externa experter kopplad till SKB:s radionuklidtransportmetod är, till viss del, beroende av SKB: s svar på frågor som tagits upp i den pågående granskningen och resultat av det arbete som identifierats för den kommande granskningsfasen. Ändå rekommenderar vi ytterligare kontroller av koder och data som används samt av genomförda beräkningar i SR-Site.

Appendix i denna Technical Note innehåller:

- specifika önskemål om förtydliganden och ytterligare arbete av SKB;
- lista på specifika frågor som kräver ytterligare granskning och analys av SSM och dess externa exporter; samt
- två oberoende beräkningar för att testa vissa påståenden som SKB gjort i de granskade rapporterna.

Projektinformation
Kontaktperson på SSM: Shulan Xu
Diarienummer ramavtal: SSM2011-4246
Diarienummer avrop: SSM2012-140
Aktivitetsnummer: 3030007-4028

SSM perspective

Background

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

Objectives of the project

The objective of this review task is to consider whether SKB's methodology to abstract FEPs (features, events, processes) and site information as well as other data into assessment models for radionuclide transport is appropriate and sufficient for its purpose. In particular, it shall be analysed if SKB's technical arguments are sound, appropriate and adequate to support the results and conclusions.

Summary by the authors

As part of SSM's Initial Review Phase of SKB's SR-Site safety assessment of the final disposal of spent nuclear fuel at the Forsmark site, Quintessa has been requested by SSM to consider whether SKB's methodology to abstract FEPs (features, events, processes), as well as site information and other data, into assessment models for radionuclide transport is appropriate and sufficient for its purpose. This Technical Note summarises the findings of Quintessa's review.

The reviewers consider that SKB's methodology appears to be appropriate and sufficient but there is scope for improvements to be made in the clarity of its documentation. Information relevant to the radionuclide transport methodology is dispersed around various reports rather than being summarised in a single high level report, which then references supporting detailed reports. The transparency and traceability of the reports is further hindered by the reports rarely providing section numbers when citing other SR-Site reports, and by the preponderance of probabilistic calculations, which makes it much more difficult for the reader to gain a good understanding of what really matters (averaging over a large number of realisations hides important features of the calculations) and hinders the reproduction of SKB's calculations by a third party.

The completeness and scientific soundness and quality of the work reviewed are considered to be generally good. The reviewers particularly welcome the use of analytical and simplified models to complement the use of numerical models. However, the review has identified:

- limited information on certain aspects of the methodology such as the process of developing conceptual models using FEPs and site information;
- limited justification for the inclusion/exclusion of FEPs in the reviewed reports;

- some gaps in the calculation cases considered;
- certain quality assurance issues associated with the data and calculations reviewed; and
- issues over the adequacy of the gas calculations.

The need for further review and analysis by SSM and its external experts of SKB's radionuclide transport methodology is, to some extent, dependent on SKB's answers to questions raised in the current review and the results of the further work identified. Nevertheless, further checks on the codes and data used and the calculations undertaken in SR-Site are recommended.

Appendices are provided in this Technical Note covering:

- specific requests for clarification and further work by SKB;
- a list of specific issues requiring additional review and analysis by SSM and its external experts; and
- two sets of independent calculations to test certain claims made by SKB in the reviewed reports.

Project information
Contact person at SSM: Shulan Xu
Framework agreement number: SSM2011-4246
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Author: Richard Little, Philip Maul, Peter Robinson and Claire Watson
Quintessa, Henley on Thames, UK

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Content

1. Introduction

As part of SSM's Initial Review Phase of SKB's SR-Site safety assessment of the final disposal of spent nuclear fuel at the Forsmark site, Quintessa has been requested by SSM to consider whether SKB's methodology to abstract FEPs (features, events, processes), as well as site information and other data, into assessment models for radionuclide transport is appropriate and sufficient for its purpose. In particular, the soundness, appropriateness and adequacy of SKB's technical arguments to support the results and conclusions should be evaluated. This Technical Note summarises the findings of Quintessa's review.

The primary reviewed documents, where transport calculations are reported, are TR-11-01 (the main report) and TR-10-50 (the radionuclide transport report). Other supporting documents have also been reviewed as indicated in Appendix 1. Radionuclide transport issues associated with the use of the MARFA code are covered in a separate Technical Note (Robinson, 2012) and are not duplicated here.

The main review findings are presented in Section 2. Specific requests for clarification and further work by SKB are provided in Appendix 2, together with other technical and editorial observations on the reviewed reports. Key recommendations to SSM for further work are summarised in Section 3, with a list of specific issues requiring additional review and analysis by SSM and its external experts being provided in Appendix 3.

Two sets of independent calculations have been undertaken as part of the review to test certain claims made by SKB in the reviewed reports. The claim that the effects of channelling in fractures can be ignored when choosing F-factor values for radionuclide transport calculations is investigated in Appendix 4. The claim that the inclusion of Th-230 sorption in the near field is pessimistic, since it promotes ingrowth of Ra-226 in the buffer, is investigated in Appendix 5.

2. Main Review Findings

2.1. Documentation of SKB's Radionuclide Transport Methodology

The reviewers were expecting there to be a well-explained and documented process in the SR-Site reports showing how FEPs and site information were incorporated into the conceptual and mathematical models of radionuclide transport, and then into the software tools and associated calculation cases. However, the reports do not provide such clear documentation and the process is not synthesised in the **main report** (TR-11-01) in a manner that facilities reviewing and auditing. Information relevant to the methodology is dispersed around various SR-Site reports so it was necessary to review a number of reports in order to develop an understanding of the approach used.

As a starting point, the **FEPs report** (TR-10-45) was reviewed in order to understand the key FEPs. The report provides a somewhat repetitive description of the detailed process followed in undertaking the extensive and impressive FEP audit. Unfortunately, limited details are provided in the report itself of the reasons for the inclusion/exclusion of FEPs from the SR-Site FEP catalogue – the reader has to go to each individual process report in order to gain further information. The only exception is Section 4.3.4, where there is a very useful explanation and justification for the exclusion of the "meteorite impact" FEP that cites relevant references. The reviewers also found that the descriptions of the FEPs are limited in TR-10-45. It had been hoped that further details, including reasons for the inclusion/exclusion of FEPs, would be provided in the electronic copy of the SR-Site FEP catalogue but that was not the case.

Site information is provided in the **site description report** (TR-08-05), the review of which is beyond the scope of the current project, and appears to be adequately synthesised in Chapter 4 of TR-11-01. The conceptual models for radionuclide transport developed using the FEPs and site information are described in the individual process reports (for example the **geosphere process report** (TR-10-48)) and summarised in Chapter 3 of the **radionuclide transport report** (TR-10-50). In general, these reports provide a reasonably good description of the key processes, although more details would be helpful for certain processes (see for example comments on TR-10-48 and TR-10-50 in Appendix 2 of this Technical Note). However, the process of taking the FEPs and site information to develop the conceptual models is not clearly explained or documented. The documentation of the process could be improved by developing a table that lists each FEP from the SR-Site FEP catalogue and explains how it is incorporated into the conceptual model(s) with cross references to the relevant sections in the process reports and the site description report. If a FEP is not included in the conceptual model(s), the reasons/justifications for its exclusion could be given in the table.

The incorporation of the conceptual models for radionuclide transport and their FEPs into the software tools (COMP23, FARF31 and MARFA) is documented in Section 13.4.1 and 13.4.2 of TR-11-01 and repeated in Sections 3.6.1 to 3.6.3 of TR-10-50. The adequacy of the documentation could be improved by developing a table that lists each FEP affecting radionuclide transport from the SR-Site FEP catalogue and explains how it is incorporated into each software tool with

appropriate cross references to the sections in the relevant software reports. If a FEP is not included in a particular software tool, the reasons/justifications for its exclusion could be given in the table. A further improvement would be the provision of a table summarising the calculation cases undertaken for radionuclide transport and the codes used since it is not always apparent which radionuclide transport code(s) have been used for which case(s). The table could summarise the motivation for each calculation case.

Transport parameters reported in the **data report** (TR-10-52) were reviewed. Section 1.1 of TR-10-52 states that: "This report compiles, documents, and qualifies input data identified as essential for the long-term safety assessment of a KBS-3 repository…". However, the report does not contain all the data that are required for transport calculations. Furthermore, the data that are included are described and justified at variable levels of detail. For example, little information is given about the compositions of the buffer and backfill materials; instead readers who seek detailed information are referred to the **buffer production report** (TR-10-15) and the **backfill production report** (TR-10-16). In contrast, there is a detailed description in Section 5.3 of TR-10-52 of the approach to selecting Kd values in buffer and backfill materials which is presented in a complex and often unclear manner, thereby making it difficult for the reader to form an opinion about data quality.

2.2. Justification for Inclusion/Exclusion of FEPs

Limited details are provided in TR-10-45 and the SKB FEP database of the reasons for the inclusion/exclusion of FEPs from the SR-Site FEP catalogue. The audit of SR-Site FEPs against NEA Project FEPs in the appendices of the report does provide some limited discussion of the reasons for the exclusion of certain FEPs. However, the text is limited to a sentence or two and no justification and references are provided for the exclusion of the FEPs.

Some further evidence is provided in Chapter 6 of TR-10-48; however it too is often limited and does not meet the aim of document. For example the TRUE-1 and TRUE Block scale experiments are mentioned in only two sentences in Section 6.1.4, the second of which states "In short, the TRUE experience indicates an adequate understanding of the relevant processes" but provides no evidence of this. The reader would have to examine the nine cited reports to verify that this was the case. At the very least, the evidence in the reports should be summarised in Section 6.1.4. The same section also makes the unsubstantiated comment that "the type of processes that typically dominate tracer experiments … are not necessarily of interest on the longer timescales".

Section 2.4 (Transport and retention process) of TR-10-50 has a short paragraph on the processes included in SR-Site followed by eight pages of text on the exclusion of some processes. However, the exclusion of certain radionuclide transport processes does not appear to be documented, for example the diffusion of radionuclides along fractures and the release of radioactive gases into the biosphere due to dissolution of gas in the shallow geosphere.

In summary, the justification that is provided for the inclusion/exclusion of FEPs in SR-Site appears to be distributed around a number of documents rather than in a single document which hinders the review and auditing of the process. Furthermore,

the SKB FEP database does not provide a central repository of the reasons for the inclusion/exclusion of FEPs.

2.3. Representation of FEPs

2.3.1. Gas Releases

The focus of SR-Site is understandably on the release and transport of radionuclides in the liquid phase rather than the gas phase. However, it is somewhat surprising that there are only two pages in TR-11-01, no pages in TR-10-50 and four pages in TR-10-48 relating to the potential transport of radionuclides in the gas phase. Furthermore, the calculations presented are only for C-14 and Rn-222; no justification is given for the exclusion of Cl-36, Se-79 and I-129 (which can occur in gaseous form) from the gas calculations.

A simple model for gas release from a canister direct to the biosphere is adopted. The model is described in Section 13.8 of TR-11-01 and assumes that, on failure of the canister, 50% of the C-14 and Rn-222 inventory is immediately released to the biosphere (there is no account taken of transport through the geosphere). However, there is no justification given for the selection of the 50% value. The gas doses in Table 13-11 of TR-11-01 are supposed to be taken from a SR-Can report (R-06-82). The C-14 ingestion and inhalation doses and the Rn-222 outdoor inhalation dose given in Table 13-11 are a factor of 50 lower than those given in R-06-82 and the Rn-222 indoor inhalation dose is a factor of 32 lower. This difference appears to arise from the doses in TR-11-01 being "annual mean life time" doses, i.e. the doses calculated in R-06-82 are averaged over 50 years to obtain annual average lifetime doses reported in TR-11-01 (see 2nd paragraph on page 108 of R-06-82). This difference is not noted, explained or justified in TR-11-01. Furthermore, it does not explain the factor of 32 difference in the Rn-222 indoor inhalation dose between TR-11-01 and R-06-82.

R-06-82 in turn cites R-06-81. Examination of both reports highlights the following additional issues with the calculations.

- Both R-06-81 and R-06-82 use a Rn-222 release of 25 GBq which is considered to represent 50% of the inventory at 100,000 years. Calculations using AMBER (Quintessa 2011) and data from Tables 3-5 and 3-7 of the **data report** (TR-10-52) show that the Rn-222 inventory at 100,000 years is around 91 GBq and so a release of about 45 GBq (rather than 25 GBq) should be considered. Furthermore, the peak Rn-222 inventory (about 110 GBq) does not occur until around 200,000 years and so a peak release of about 55 GBq (more than twice the release evaluated in R-06-81 and R-06-82) could be considered.
- Calculations using AMBER (Quintessa 2011) and data from Tables 3-5 and 3-7 of TR-10-52 show that the C-14 inventory at 10,000 years is 25 GBq and so the release should be 12.5 GBq rather than 10 GBq release evaluated in R-06-81 and R-06-82.
- R-06-81 gives a C-14 ingestion dose of 1.3 µSv/a whereas R-06-82 gives an equivalent dose of 1.8 µSv/a. This is due to the change in the carbon content of the air from 0.176 g/m^3 in R-06-81 to 0.13 g/m^3 in R-06-82 (which is actually consistent with the text on p 37 of R-06-81). This change is not brought to the reader's attention in R-06-82 or in TR-11-01.

- Both R-06-81 and R-06-82 use a factor for local production of 0.1 for the calculation of C-14 ingestion dose, whereas the reviewers believe this should be 0.01 (i.e. the ratio of the area of release, 10^4 m^2, to the area considered in UNSCEAR (1988) , 10^6 m^2). Using a value of 0.01 would reduce the C-14 ingestion dose by an order of magnitude.
- The text in the 1st paragraph of Section 7.1 of R-06-81 suggests a release period of "some days to several ten days". Adopting a value of 10 days rather than the 365 days adopted in Table 7-1, results in a C-14 ingestion dose of 6.6 µSv (assuming a local production factor of 0.01).
- The values for the area of release (10^4 m^2) and height of the mixing layer (20 m) are not justified in any of the reports. If more conservative values of 10^3 m^2 and 2 m are adopted, then the C-14 ingestion dose increases by a further factor of three to 21 µSv (i.e. above the risk limit). This dose assumes a release period of 10 days and a local production factor of 0.01. Assuming 10^3 m^2 and 2 m results in outdoor doses for C-14 and Rn-222 increasing by a factor of about 30, resulting in a Rn-222 dose of 166 µSv/a (more than an order of magnitude above the risk limit).
- Equation 7.2 in R-06-81 should have ΔT in the denominator. The calculations presented in R-06-81 for outdoor inhalation doses have been undertaken with ΔT in the denominator and so are numerically correct.
- R-06-81 gives a Rn-222 outdoor inhalation dose of 5.3 µSv/a (consistent with the data given in the report and assuming ΔT in the denominator of Equation 7.2) but R-06-82 (which cites R-06-81) gives a dose of 11 µSv/a (inconsistent with the data given in the report). This modification is not brought to the reader's attention or explained in R-06-82.
- Equation 7.3 in R-06-81 should have ΔT (in units of hours) in the denominator. The calculations presented in R-06-81 for outdoor inhalation doses have been undertaken with ΔT in the denominator and so are numerically correct.
- It could be argued that the values for the ventilation rate (2 h^{-1}), building volume (1000 m^3) and the occupancy factor (0.5) used for the indoor inhalation dose calculations are not appropriately conservative. If more conservative values of 0.35 h^{-1} (Garisto et al., 2004), 300 m^3 (single story dwelling) and 1.0 (appropriate for house dweller in winter) were adopted, doses would increase by almost a factor of 40.

2.3.2. Solubility Limitation

Appendix F of TR-10-50 gives details of how solubility limits have been calculated. Review of this appendix has identified a number of issues.

First, although varying the thermodynamic data appears to be the most important contribution to variability in the solubility limits, no quantitative consideration is given in Appendix F to the variation of solubility limits with temperature; all the calculations were for 25 °C. Significantly lower temperatures can be expected under permafrost and glacial climate conditions.

Second, it is interesting to note that the solubility distributions employed in SR-Site for some radionuclides appear to differ markedly from those employed in SR-Can. It would have been helpful if SKB had discussed the reasons for these changes.

Third, it is stated in Appendix F.4 that: "*COMP23 does not allow changes in solubility limits with time. Therefore, a mixture of groundwater compositions*

representing the entire time period was used to calculate one set of solubility limits for the safety assessment. Since the uncertainty in thermodynamic data appears to have a larger impact on the solubility limits than variations in groundwater composition, the choice of groundwater should be of less importance. The solubility limits for the safety assessment were thus calculated with a groundwater composition consisting of 25% of groundwater compositions representing the temperate climate, 25% representing the permafrost climate, 25% representing glacial climate and 25% representing submerged climate."

This would appear to be a potentially important shortcoming of COMP23 as it is not possible to investigate how fluxes from the near field change with the glacial cycle. Other codes capable of undertaking the types of calculations undertaken by COMP23 (e.g. AMBER) would have no problem with this time variation. The justification given by SKB for the approximation employed is not considered to be adequate.

In the context of the overall assessment, it is the solubilities of U, Th and Ra that are important. Contrary to SKB's statement, the variation of Ra solubility with climatic conditions (Figure F-4) would appear to be potentially important.

This example also illustrates that some decisions appear to be taken because of what SKB's codes can do, even when a relatively minor change would have allowed a better model to be used.

2.3.3. Sorption

Two limitations with the treatment of sorption in SR-Site have been identified.

First, the nature and validity of the Kd concept and the limitations on its application are not discussed in the SR-Site reports. The limitations of the Kd concept are discussed in a number of sources to which reference should have been made (e.g. McKinley and Alexander, 1993). The use of Kd assumes that there are an infinite number of sites on a sorbing surface at which a particular specie may sorb. In reality there will be a finite number of such sites. The Kd concept is therefore valid only if the sorbent has not been "saturated" with the sorbing species. Sorption isotherms, such as Langmuir isotherms are conceptually closer to reality. There should be a discussion of the advantages and limitations of the Kd concept within TR-10-52, but none is given.

Second, it is stated in Section 5.9 of TR-10-48 that if the uptake of radionuclides on colloids is reversible then the impact will likely be negligible whereas irreversible sorption gives a significant potential impact. The basis for this claim is not clear - surely it depends on what fraction of the radionuclides are sorbed onto colloids, not how long they stay on a particular colloidal particle? There is a statement that there are few data to determine whether or not sorption should be treated as reversible. The rapid reversible sorption/desorption approach is used in SR-Site. It is not clear where the justification for this is recorded. The reviewers note that irreversible sorption is not included in the compliance calculations in SR-Site based on arguments in the Buffer, Backfill and Closure Processes Report (TR-10-47); presumably Section 3.5.11 of that report is intended. TR-10-47 gives details of the erosion modelling work but nothing of particular relevance to radionuclide transport.

2.3.4. Transport under Periglacial and Glacial Conditions

Permafrost is explicitly identified in Table 1-4 of TR-10-48 (Ge2) as a FEP that can impact the geosphere and some account of its impact on groundwater flow is taken into account (see for example Section 2.1.2 of TR-10-50). However, its potential impact on radionuclide migration is not mentioned in Table 6-1 of TR-10-48. Section 6.1.7 of TR-10-48 states: "*Radionuclide transport during the periglacial climate domain is handled in a simplified manner. The pathlines obtained in the groundwater flow simulations for temperate conditions are used, but advective travel time and flow-related transport resistance are scaled based on the flow ratio between the periglacial- and temperate flow simulations. In addition, Kd-values and colloid concentrations are chosen to reflect the groundwater chemical conditions of the periglacial climate domain*."

However, this approach raises questions of whether pathlines obtained using groundwater flow simulations for temperate conditions are appropriate to use under periglacial conditions when permafrost is present (a similar approach is used for the glacial climate domain and so similar questions arise). Indeed, Section 6.2.4 of the **biosphere report** (TR-10-09) notes that: "*the flow paths from a repository in a periglacial climate domain will deviate from flow paths developed under present climate conditions*." It would be helpful if further justification could be given for the use of temperate pathlines under periglacial and glacial conditions.

2.3.5. Geosphere Biosphere Interface

Radionuclide transport in the geosphere and biosphere are treated using different codes. Radionuclide fluxes calculated using FARF31 and MARFA are converted into doses using landscape dose conversion factors (LDFs) derived from Pandora, as described in Section 8.7 of TR-10-09. It is important to ensure that the interface between the geosphere and biosphere and its associated processes are represented in an appropriate manner in these codes. Geosphere-biosphere interface issue are discussed further in Section 3.3.3 of Quintessa's review of landscape models used in SR-Site (Egan et al. 2012).

2.4. Radionuclide Transport Data

Each sub-section of TR-10-52 follows the same style, with a specification, experience from SR-Can, etc. ending with recommendations for what to use in SR-Site. This approach allows all the key issues to be discussed and is done in a way that brings in many issues from different disciplines. Section 5.3, which covers the migration data for the buffer and backfill, and Sections 6.7 and 6.8, which cover the migration data for the geosphere (flow related and otherwise), were reviewed.

The following questions arose from the review (additional questions/comments are given in Appendix 2):

- Were the various discrete fracture network (DFN) models presented in Section 6.6 intended to cover uncertainty for both flow and transport behaviour? The DFN models are important for specifying both the conditions around the deposition holes and transport times to the biosphere for radionuclides. Is it possible to specify alternative (more conservative) conceptual models consistent with the available data that would give higher radiological consequences?

- It is surprising that there is no attempt to justify the parameter choices for geosphere migration through any site-specific observations. Are there any site data which could be used to validate transport properties?
- What is the rationale for recommending very wide ranges of Kd values for many elements, rather than recommending conservative values? The quoted ranges of Kd are often larger than ranges that have been recommended for use in safety assessments in other programmes and could give rise to non-conservative results when applied in transport calculations.

Section 13.5.11 of TR-11-01 identifies that the key parameters affecting risks are: the time of failure of the canister(s) ($t_{Failure}$); the fuel dissolution rate (D_{fuel}); the transport resistance along the geosphere flow path (F); and the advective travel time (t_w). However, it is also important to recognise that risks are dependent on the number of canisters that are assumed to fail and so SKB's claims made for canister integrity need to be carefully reviewed, in addition to the assumptions for $t_{Failure}$, D_{fuel}, F and t_w. As for SR-Can, the number of failed canisters calculated is very low even when advective conditions are assumed in all deposition holes (see Figure 12-18 in TR-11-01). Review of all of these parameters, with the exception of F, are beyond the scope of the current radionuclide transport methodology review.

Unlike SR-Can, F has not been reduced by a factor of 10 to account for channelling. The justification for this is given in Appendix A of TR-10-50 and independent calculations have been undertaken to test the justification (see Appendix 4 of this Technical Note). The independent calculations support the findings of SKB, showing that, whilst channelling can lead to earlier breakthrough times, the effect is negligible if flow is through multiple small channels in the fracture (the most likely case for real fractures), and diminishes as F (calculated by assuming uniform flow through the whole fracture) increases.

The review of Appendix A, identified the following quality issues (see Appendix 4 of this TN).

- Not all parameters required for the calculations were given in Appendix A and in some cases it was unclear what values were used in the original calculations.
- A mixture of different units was used, in particular years and seconds.
- In one case conflicting information was given in the text and in figures (the definition of the parameter W_s).
- It was not always clear, when talking about apertures, whether the full or half aperture was meant, or similarly the width of a single stagnant zone or the total width of both symmetrically flanking zones.
- A formula included in an illustration (Figure A-5) was incorrect.
- Using a single set of input parameters it was not possible to match all of the SKB results, but nowhere was the full parameter set given, nor an indication given that it had changed

In Sections 5.3.5, 5.3.6 and 5.3.7 of TR-10-52 many uncertainties are raised in the mind of the reader because the stated assumptions and/or rationale for making choices among different data sets are not well-justified. In many places "proposals" are made for selecting data, leaving the reader to wonder what was actually done in the assessment. It would have been more appropriate to specify clearly values for use in the assessment and then discuss their associated uncertainties. Furthermore, in some places data are recommended to precisions that are not really justified given the overall uncertainties. This is the case for diffusivities. In other places very broad statements are made about uncertainties without explaining their significance. For

example, page 165 gives best estimate De values of 1.4 x 10^{-10} m^2/s for the buffer (ρd = 1,562 kg/m^3) and 1.6 x 10^{-10} m^2/s for the backfill (ρd = 1,504 kg/m^3). Given that the difference between these values is small compared to the large scatter in the De data shown in Figure 5-6, it is unjustified to recommend different values for the backfill and the buffer.

2.5. Radionuclide Transport Calculations

2.5.1. Analytical and Simplified Calculations

As well as numerical calculations, analytical calculations have been undertaken for radionuclide transport in SR-Site. The reviewers have previously supported their use and SKB's work in this area is impressive. The reviewers support the continued use of these methods and welcome the agreement with the FARF31 calculations presented in Section 4.10 of TR-10-50.

Simplifying the modelling even further has been undertaken by making use of regression models, which are described on page 691 of TR-11-01 and page 70 of TR-10-50. The more complex regression models fit the full calculations very well. The dependence of the potential consequences on the key parameters reflects what is already known, but is still useful. The approach taken here is consistent with 'insight modelling' that has been employed in other safety assessments. As indicated in the conclusions to Section 4.4.3 of TR-10-50, the relatively simple functional form employed is possible because of the simple conceptual model for the system in this scenario with no buffer and with the near-field release controlled only by the fuel dissolution rate. This is presumably why such a 'tailored' regression model has not been presented for the other scenarios that have been considered. It would be useful to know if SKB has considered this.

It is stated in the summary of TR-10-50 that the agreement between the numerical and analytical results "demonstrates that potential doses are controlled by relatively simple processes that are straightforward to understand and model". The reviewers consider that it would be more accurate to say that the agreement shows that "SKB's conceptualisation of the system and its processes results in potential doses being controlled by relatively simple processes that are straightforward to understand and model".

LDFs are used for converting releases from the geosphere to annual doses. These are derived from detailed modelling of the biosphere as described in TR-10-09. In keeping with the use of analytical and simplified calculations for the near field and geosphere, it would have been useful if some simplified calculations had been undertaken for the biosphere, for example a simple dose from drinking water calculation which could be used as a benchmark against which to compare the LDFs.

2.5.2. Deterministic Calculations

It is understandable that there is a preponderance of probabilistic calculations in the presentation of the assessment given that the regulations are expressed in risk terms. However, it makes it more difficult for the reader to gain a good understanding of what really matters (averaging over a large number of realisations hides important

features of the calculations) and hinders the reproduction of SKB's calculations by a third party. A reasonable number of deterministic calculations are presented in Section 4.4.1 of TR-10-50, but more might have been helpful and these are generally not reproduced in TR-11-01 (only Figures 13-15 and 13-16 give deterministic doses). For example, calculations for the pinhole scenario (TR-11-01, Section 13.7.2) go straight into probabilistic mode, with no deterministic calculations to help the reader.

An example of the need for more deterministic calculations relates to the distance from the deposition hole to the fracture. This distance is one of the outputs from the hydrogeological modelling and is therefore different in each case in the probabilistic calculations. This is one reason why it is difficult to reproduce the SR-Site calculations – the SR-Site documentation does not give details of the calculated values of this quantity. This leads to a lack of transparency as a third party cannot reproduce the calculations. Furthermore, large distances calculated for Forsmark might be one of the reasons that, for many calculations, radionuclides released from the near-field do not reach the biosphere.

It was suggested in Quintessa's review of SR-Can (Maul et al., 2007) that, for each set of probabilistic calculations undertaken in support of comparisons with regulatory criteria, a deterministic case should be documented to illustrate the key points. In addition, the review suggested that further insight into the important features of probabilistic calculations can be obtained by analysing the high consequence runs. Neither of these suggestions appears to have been fully adopted for SR-Site.

2.5.3. Presentation and Discussion of Results

A wide range of deterministic and probabilistic transport results are presented in TR-11-01 and TR-10-50. However, not all results are discussed in appropriate detail so the reader can be left with unanswered questions and uncertainty as to whether SKB has a full understanding of the processes affecting the results presented. For example, there is no explanatory text presented with Figure 13-50 in TR-11-01; the text simply states: "The modelling of the dose consequences in the two time frames are compared in Figure 13-50". No reference is provided to Section 5.5 of TR-10-50 where the same figure is reproduced with appropriate explanatory text.

The mean annual effective dose is plotted on all result graphs for probabilistic cases. However, only two figures (Figures 4-6 and 6-50 of TR-10-50) provide any information on associated percentiles and so it is difficult for the reader to develop an understanding of the range in the results and therefore the associated uncertainties.

2.5.4. Calculations Beyond 1 Ma

It is recognised that the regulations require consideration of risks up to one million years and so SKB understandably focusses on that time period. There is a brief (two page) qualitative account of the time period beyond one million years in Section 14.5 of TR-11-01 but no quantitative results are presented.

The reviewers consider that extending some calculations beyond one million years would be useful, especially for those cases which show risks still steeply rising at

one million years. It is recognised that over such long time periods the reliability of quantitative predictions diminishes due to growing uncertainties but it would still be useful to present some results for such timescales in order to show when impacts might peak. Graphs showing results beyond one million years could use a grey background for the period beyond one million years to emphasize the illustrative nature of the results over such timescales (see for example Nagra 2002).

In cases where risks are still rising after one million years, SKB should make it clear that the risk is a maximum risk (over the one million year time period) rather than a peak risk since the peak will occur after one million years.

2.5.5. Quality Assurance

It is somewhat worrying that a number of (minor) errors were identified with the radionuclide transport calculations at a late stage in the assessment (see Section 3.7.3 of TR-10-50). This suggests that quality assurance checks were carried out *after* the calculation process rather than *during* the process.

The checks, undertaken as part of the current review, on the gas calculations and calculations supporting the choice of the transport resistance along the geosphere flow path (*F*) have also uncovered some apparent quality assurance issues (see Section 2.3.1 and 2.4).

2.6. Editorial

The reviewers were expecting the main report (TR-11-01) to provide a high-level overview of the SR-Site project rather than a 893 page document that considers some issues in great detail (rather than summarising key points and referencing out to supporting documents) and other issues very briefly (with inadequate referencing of supporting detailed documents). The current approach does not facilitate the readability of the main report.

The readability of the SR-Site reports is further affected by much material being repeated between the reports and even within the same report. For example, the last paragraph of Section 2.1 and the first paragraph of Section 2.1.2 in TR-10-50 are essentially the same, even though they are separated by only a page.

When information from another SR-Site report is cited, it is rare that the relevant section number is cited. This hinders the reader's ability to cross-check the information. For example Section 2.2 of TR-10-45 notes that Step h of the FEP processing produced is described in the TR-11-01 but does not give the relevant section number. This issue even arises in the same document. For example, it is noted in Section 1 of TR-10-50 that the report provides details on several radionuclide transport/retention processes that are not explicitly included in SR-Site but require further analyses. However, no forward reference is given to the relevant section.

2.7. Summary of Findings

SSM has suggested that all the reviewers should consider the following issues in their review of the relevant SR-Site reports as they relate to the scope of the review:

- the completeness of the documented work;
- the scientific soundness and quality of the documented work;
- the adequacy of relevant models, data and safety functions;
- the handling of uncertainties;
- the safety significance of the work; and
- the quality in terms of transparency and traceability of information in the reports.

The findings relating to these issues for the review of SKB's radionuclide transport methodology are summarised in Table 1.

Table 1: Summary Findings of the Review of SKB's Radionuclide Transport Methodology used for SR-Site

Issue	Finding
Completeness	**Generally good**, although limited documentation is provided for the inclusion/exclusion of FEPs from the SR-Site FEP catalogue (see Section 2.2) and the process of developing conceptual models using FEPs and site information (see Section 2.1). Although a wide range of calculation cases has been evaluated for radionuclide transport, not all results are discussed in appropriate detail (Section 2.5.3). Furthermore, there are some gaps in the cases considered. For example: • limited consideration is given to gas release (Section 2.3.1); • consideration of changes in Ra solubility limits with time (see Section 2.3.2); • irreversible sorption on colloids is not included in the compliance calculations (see Section 2.3.3); • consideration of pathlines under periglacial and glacial conditions (see Section 2.3.4); and • calculations beyond one million years have not been considered; such calculations would be useful, especially for those cases which show risks still steeply rising at one million years (see Section 2.5.4).
Scientific soundness and quality	**Generally good**, although quality assurance issues have been identified with certain calculations (see Section 2.5.5). Furthermore, the documentation of the approach used and the associated assumptions/decisions lacks clarity and is variable in its level of detail (see Section 2.6). This can sometimes make it difficult to evaluate their scientific soundness.
Adequacy of relevant models, data and safety functions	**Generally good**, especially given that analytical and simplified models are used in addition to numerical models (see Section 2.5.1). Some relatively minor updates to codes could have been made (e.g. time-dependence in COMP23 solubility – see Section 2.3.2) to avoid some forced approximations. **T**here are also issues over the adequacy of the gas calculations (Section 2.3.1), as well as concerns expressed in Robinson (2012) about the quality assurance of the MARFA code. Furthermore, it is considered that assumptions and/or rationale for making some choices among different data sets for radionuclide transport calculations are not well-justified (see Section 2.4).
Handling of uncertainties	**Generally good**: a range of calculation cases have been evaluated for radionuclide transport that allow the investigation of conceptual, model and data uncertainties using both deterministic and probabilistic approaches. However, the SR-Site documentation would benefit from an explicit section in the main report that summarise the approach taken to manage uncertainties in SR-Site. In addition, as noted in Section 2.5.3, percentiles as well as mean values should be shown on graphs for the key probabilistic cases.

Issue	Finding
Safety significance	**Limited**: as noted in Section 2.4, the safety of the repository is primarily dependent on: the number of canisters that fail; the time of failure; the fuel dissolution rate; the advective travel time; and the transport resistance along the geosphere flow path. Only the last item is within the scope of this specific review and the review has shown that SKB's work relating to this parameter is generally adequate (subject to some observations) (see Section 2.4). Kd values have some (secondary) impact on risks and, as noted in Section 2.4, the ranges of Kd could give rise to risk dilution when applied in transport calculations.
Quality in terms of transparency and traceability of information	**Poor**: information relevant to the radionuclide transport methodology is dispersed around various reports and described in differing level of detail rather than being summarised in a single high level report that then references supporting detailed reports (see Sections 2.1 and 2.2). All the reports need to be read in order to try and develop an understanding of the approach used. Transparency and traceability is further hindered by the reports rarely providing section numbers when citing other SR-Site reports (see Section 2.6) and by the limited number of deterministic calculations (see Section 2.5.2). Similar problems are encountered with the radionuclide transport data; the data report does not contain all the data that are required for transport calculations and the data that are included are described and justified at variable levels of detail (see Section 2.1).

3. Recommendations to SSM

Key issues associated with SKB's radionuclide transport methodology have been raised in Section 2 and specific requests for clarification and further work by SKB are listed in Appendix 2. It is recommended that these be addressed in the first instance by seeking responses from SKB.

In addition, when referring to the regulatory review of SR-Can, SKB state on page 54 of TR-11-01: "*All conclusions from the review have been considered in detail in the preparation of this report.....The review findings have been used to identify a large number of items that are addressed in a structured way in the SR-Site assessment. The documentation of these items and their handling in SR-Site forms part of the project documentation and is made available to reviewing authorities on request, but is not issued as an SKB report".* If SSM has not already done so, it is recommended that it request this documentation and undertake an audit to ensure that the SR-Can review comments have been appropriately addressed in the SR-Site reports.

The need for further review and analytical work by SSM and its external experts is, to some extent, dependent on the answers to questions raised in Appendix 2 and the results of the further work to be undertaken by SKB identified in Appendix 2. Nevertheless, it is already considered that further checks on the codes and data used and the calculations undertaken in SR-Site should be undertaken. A proposed preliminary list of specific topics relevant to SKB's radionuclide transport methodology, which require additional work by SSM and its external experts, is provided in Appendix 3.

References

Bastug, T. and Kuyucak, S (2005). Temperature dependence of the transport coefficients of ions from molecular dynamics simulations. Chemical Physics Letters, 408, 84–88.

Bradbury, M and Baeyens B (2002). Near field sorption data bases for compacted MX-80 bentonite for performance assessment of high-level radioactive waste repository Opalinus Clay host rock. Paul Scherrer Institute Report PSI Bericht 03-07.

Egan, M.J., Little, R.H. and Walke, R.C. (2012). Review of Landscape Models Used in SR-Site. SSM Technical Note, Procurement reference SSM2011-4543, Activity Number 3030007-4034.

Garisto, F., D'Andrea A., Gierszewski P. and Melnyk T. (2004). Third Case Study – Reference Data and Codes. Ontario Power Generation Report OPG 06819-REP-01200-10107-R00. Toronto, Canada.

Maul, P.R., Robinson, P.C., Bond, A.E. and Benbow, S.J. (2007). Independent Calculations for the SR-Can Assessment. SKI Report 2008:12.

McKinley, I.G., and Alexander, W.R. (1993). Assessment of radionuclide retardation: uses and abuses of natural analogue studies. Journal of Contaminant Hydrology, 13, 249–259.

Nagra (2002). Project Opalinus Clay: Safety Report, Demonstration of the Disposal Feasibility for Spent Fuel, Vitrified HLW and Long-lived ILW. Nagra Technical Report 02-05. Wettingen, Switzerland.

Quintessa (2011). AMBER 5.5 Reference Guide. Quintessa Ltd. Report QE-AMBER-1, Version 5.5. Henley-on-Thames, United Kingdom.

Robinson, P.C. (2012). Review of the MARFA Code. SSM Technical Note, Procurement reference SSM2011-592, Activity Number 3030007-4029.

UNSCEAR (1988). Report to the General Assembly, 1988. United Nations, New York.

Appendix 1: Coverage of SKB reports

The SKB reports covered in this review are given in Table A1. These include all the mandatory SKB reports specified in the assignment together with two reports that include discussion of the gas release calculations (R-06-81 and R-06-82).

Table A1: SKB Reports Reviewed

Reviewed report	Reviewed sections	Comments
TR-11-01 (Main report)	Sections 13.4–13.8, 14.5	
TR-10-50 (Radionuclide transport report)	Entire report including appendices	
TR-10-51 (Model summary report)	Sections 3.9, 3.12 and 3.20	These sections cover FARF31, COMP23 and solubility model
TR-10-45 (FEPs report)	Entire report including appendices	Focussed on radionuclide transport FEPs
SKB FEP database	SR-Site FEPs	Focussed on radionuclide transport FEPs
TR-10-48 (Geosphere process report)	Chapter 1, Section 5.9, Chapter 6	Colloidal processes and radionuclides transport processes
TR-10-52 (Data report)	Sections 5.3, 6.7 and 6.8	Migration properties in buffer, backfill and geosphere. Other parameters affect radionuclide migration (e.g. canister failure times and fuel dissolution rates) but these are beyond the scope of the Quintessa review.
R-06-81 (SR-Can ecosystem models report)	Chapter 7	Gas release calculations
R-06-82 (SR-Can biosphere report)	Section 8.2.4	Gas release calculations

Appendix 2: Suggested requests for additional information from SKB

This appendix provides a list of requests for additional information from SKB arising from the review of each report. The requests are differentiated into:

- requests for clarification from SKB of existing information presented in the SR-Site reports; and
- requests for further work by SKB to clarify existing information or rectify omissions in the SR-Site reports.

Note that the list of requests for further work might increase in light of SKB's responses to the requests for clarification.

In addition to the requests for clarification and further work, other technical and editorial observations are provided on each reviewed report.

TR-11-01

Key Requests for Clarification

1. None.

Other Requests for Clarification

1. Section 13.5.3, 4th para: What is the basis for increasing q by a factor of two to account for the locally increased flow due to the void from the eroded buffer?
2. Section 13.5.8, 1st bullet: The reviewer presumes that there are no Swedish activity constraints and so Finnish constraints are used. Is this the case?
3. Section 13.6.2, p 696, 4th para: Should "0.28 μSv" read "4.2 μSv"?
4. Section 13.8, 3rd para: Where is evidence provided in the suite of SR-Site documents that hydrogen is sufficiently soluble in water to be carried away by the advective flow?
5. Section 13.8, 4th para: What is the justification for assuming that half the inventory of C-14 and Rn-222 is released immediately? Why not assume 100% for the purpose of the scoping calculation?
6. Table 13-11: Why are the C-14 ingestion and inhalation doses and Rn-222 outdoor inhalation dose a factor of 50 lower than those given in SKB (2006g)? The reviewers believe that it is because the doses in TR-11-01 are "annual mean life time" doses, i.e. the doses calculated in R-06-82 are integrated over 50 years to obtain the annual average lifetime doses reported in TR-11-01 (see 2nd para on page 108 of R-06-82). This process is not noted, explained or justified in TR-11-01.
7. Table 13-11: Why is the Rn-222 indoor inhalation dose a factor of 32 lower than those given in SKB (2006g)?

Key Requests for Further Work

1. LDFs are used for converting releases from the geosphere to annual doses. These are derived from detailed modelling of the biosphere as described in TR-10-09. In keeping with the use of analytical and simplified calculations for the near field and geosphere, it would be useful if some simplified calculations could be undertaken for the biosphere, for example a simple dose from drinking water calculation which could be used as a benchmark against which to compare the LDFs.
2. The gas calculations represent in TR-11-01 need to be improved. There are various calculation errors and inconsistencies, and non-conservative and poorly justified/explained assumptions (see Section 2.3.1 of this TN). The text and calculations associated with the gas release and transport need to updated and revised to these concerns.

Other Requests for Further Work

1. Although the regulations do not require consideration of risks beyond one million years, the reviewers consider that extending some calculations beyond one million years would be useful, especially for those cases which show risks still steeply rising at one million years (e.g. the central corrosion case). It is recognised that over such long time periods the reliability of quantitative predictions diminishes due to growing uncertainties but it

would still be useful to present some results for such timescales in order to show when impacts might peak. Graphs showing results beyond one million years could use a grey background for the period beyond one million years to emphasize the illustrative nature of the results over such timescales (see for example Nagra 2002).

Other Observations

1. Section 13.4.1, 4th para: It would have been useful if some brief explanation could have been provided to explain why no or little EDZ would be formed around the deposition tunnel. At the very least the relevant section in TR-10-18 should have been given.
1. Section 13.5.4, 1st para: The omission of the contributions of the instantaneously released fraction in the subsequent figures should have been noted in the figure captions.
2. Section 13.5.6, 3rd para: The case of colloid facilitated transport is in fact reported on page 678 of TR-11-01. "five" should read "four".
3. Figure 13-17 (and similar figures): It would have been useful if at least the 95% confidence limits for the total dose had been shown as well as the mean dose.
4. Figure 13-22 (and similar figures): It would have been useful if the figure had been simplified to show variant case's total dose and doses for top 2 or 3 radionuclides doses plus total dose for central case.
5. Section 13.5.6, DFN model variant: Was not given in list at start of Section 13.5.6.
6. Section 13.5.6, Advection in deposition holes variant: Was not given in list at start of Section 13.5.6.
7. Figures 13-39 and 13-40: Excellent summary figures that would benefit from showing the dose for the central case.
8. Section 13.6.1, 2nd bullet: It would have been helpful to explain where evidence is provided in the suite of SR-Site documents to show that shear movement will not affect the buffer to the extent that its protection against advective flow will be impaired.
9. Section 13.6.2, p 696, 1st para: It would have been useful to have some text discussing Figure 13-50. At present it is just presented with no text.
10. Section 13.6.4, p 704, 3rd para: It would have been useful to have some text to explain how the collective dose of 4×10^{-5} manSv compares with reference levels/regulatory limits.
11. Section 13.8, 8th para and Table 13-11: SKB (2006 g and h) are cited. However, only SKB (2006g) is given in the reference list. The reviewers believe that SKB (2006h) is R-06-81.

TR-10-50

Key Requests for Clarification

1. None

Other Requests for Clarification

1. Section 2.2.2: Is the model of groundwater chemistry evolution based on the results of mathematical modelling or is it a purely conceptual model? If the former, in which section of which report is the modelling described?
2. Section 2.4.4, 3rd para: Where is the source for the approximation that matrix retardation is proportional to the square of the F-factor. Is it Appendix B?
3. Section 2.4.4, 8th para: Are there any modelling results to the support the statement that "remobilisation is generally not expected to be large even in cases where it might be reasonably expected to occur"?
4. Section 3, 2nd para: Why has the EFPC criterion been applied for most of the calculation cases?
5. Section 3.2: The first two bullet points are discussed further in Sections 3.2.1 and 3.2.2. Why aren't the last two bullet points described in subsequent sub-sections?
6. Section 3.6, 2nd para: It is stated that details of the analytical model are given in TR-10-51 but this is not the case. Where are the details provided in the SR-Site documents?
7. Section 3.6.4, 5th para: Where in the report is the model for the partitioning process described?
8. Section 3.6.4, 5th para: What is the QA status of the Mathematica scripts?
9. Section 3.7.1, 1st para: Why were 6916 iterations run? What convergence tests were undertaken?
10. Section 3.7.1, 3rd para: Why was the case with a failure at 100,000 years run with 1000? What convergence tests were undertaken?
11. Figures 4-5 and 6-50: Why are these the only two figures in the entire report that provide information on percentiles?
12. Section 4.4.3, tailored regression model: The model is referenced in external publications, but this work appears not to have been reported in SKB reports. Is this the case, and, if so, what is the reason for this?
13. Section 4.4.3, Conclusions: Why has a 'tailored' regression model not been presented for scenarios other than the canister corrosion scenario?
14. Section 4.4.4: Why is the issue of parameter correlations not discussed under this section, or at least a cross-reference to the relevant section (Section 2.3.9) in TR-10-52 provided?
15. Section 4.4.4, 1st para: Why was the dose from Ni-59 rather than Ra-226 or the total dose used for the analysis of convergence?
16. Section 4.5.5, 1st para: Why was the number of correlation groups reduced from five to two? Where is this reduction explained?
17. Appendix A.2, 2nd para: W_s is reported as being the half width of the total stagnant zone, i.e. 4.5 times the width of the flow channel. In Figure A-2, it is indicated as being the full width of the total stagnant zone, i.e. 9 times the width of the flow channel. Which is correct? Note that it was found

that the SKB calculations could only be matched if the former definition is used (see Appendix 4 of this Technical Note).

18. Appendix A.2, 4th para: what values are used for the transport porosity of rock matrix (θ_m), the bulk desnity of rock matrix (ρ_r), the free component diffusivity in fracture water (D_w)? Data do not appear to be provided in Appendix A.
19. Why is the gap between the Case 1 and Case 2 results on Figure A-7 larger than the two cases (1E5 and 1E6) that should bound it on Figure A-9?
20. Appendix B: This contains many small discussions and calculations relevant to retention properties. It is unclear whether these issues have been taken into account in the data report. How does it relate to the Kd discussions in the data report?
21. Appendix B, page 209. Upper and lower limits are both stated to be 1 mm – should the lower limit be 1 micron?
22. Appendix D: Insufficient data are provided to reproduce all the selection of radionuclides calculations given. Specifically what flux to dose conversion factors were used for the hypothetical case?
23. Appendix D, 1st para: Why is the selection of radionuclides based on SR-Can data rather than SR-Site data?
24. Appendix D.1: What flux to dose conversion factors were used for this hypothetical case?
25. Appendix D.1: Given the need for conservative calculations, why wasn't a fuel dissolution rate of 10^{-6}/y (i.e. fastest rate given in TR-10-52) used?
26. Appendix D.2, 2nd para: Why is a total hazard index of less than 0.01 Sv used? Why is the line on Figure D-1 at 0.1 Sv rather than 0.01 Sv?
27. Appendix D.3: Do the dose conversion factors for parent radionuclides used in the calculations take into account the contribution of their daughters which are assumed to be in equilibrium with the parent?
28. Appendix F: Given that varying the thermodynamic data appears to be the most important contribution to variability in the solubility limits, why is no quantitative consideration given to the variation of solubility limits with temperature (all the calculations are for 25 °C)?
29. Appendix F: It is interesting to note that the solubility distributions employed in SR-Site appear to differ markedly from those employed in SR-Can for some radionuclides. The reasons for these changes are not discussed in TR-10-50, are they provided in another SR-Site reports?
30. Appendix F.3: Do the first set of calculated solubility values given in Appendix F.3 consider uncertainties in both the groundwater compositions and the equilibrium constants? Calculations presented later in that section are for variable groundwater conditions and fixed equilibrium constants and fixed groundwater conditions and variable equilibrium constants.

Key Requests for Further Work

1. A reasonable number of deterministic calculations are presented in TR-10-50, but more might have been useful to develop understanding of key processes and facilitate the reproduction of SKB's calculations. For example, it would be useful to undertake more deterministic calculations relating to the distance from the deposition hole to the fracture. This distance is one of the outputs from the hydrogeological modelling and is

therefore different in each case in the probabilistic calculations. This is one reason why it is difficult to reproduce the SR-Site calculations – the SR-Site documentation does not give details of the calculated values of this quantity. This leads to a lack of transparency as a third party cannot reproduce the calculations. Furthermore, large distances calculated for Forsmark might be one of the reasons that, for many calculations, radionuclides released from the near-field do not reach the biosphere.

2. As noted in Section 2.3.2 of this TN, COMP23 does not allow for changes in solubility limits with time and so does not have the capability to investigate how fluxes from the near field might change as a result of climate change. SKB should undertake some assessment calculations that include the time variation of at least Ra solubilities in the near-field.
3. The mean annual effective dose is plotted on all results graphs for probabilistic cases. It would be useful to have information on the range of the results through the plotting of percentiles. Only two figures (Figures 4-6 and 6-50 of TR-10-50) provide any information on percentiles. SKB should provide additional graphs showing percentiles (e.g. 5th and 95th) for the key calculation case in order to allow the reader to develop an understanding of the range in results. In addition, an updated version of Table 7-1 of TR-10-50 should be produced giving maximum values for 5th and 95th percentiles for each calculation case.

Other Requests for Further Work

1. Section 3.6.1, 4th para: What are the limitations/implications of the use of analytical solutions, instead of fine discretisation, at sensitive zones, for example at the exit point of a small canister hole and at the entrance to fractures?
2. Section 3.7.3, 5th bullet: Results with the correct plutonium solubility limits should be provided.
3. Appendix D.3: It would be useful to have information relating to the treatment of the decay of Mo-93 to Nb-93m, and the decay of Sr-90, Ag-108m, Sn-121m and Cs-137 to short-lived daughters which can contribute to the dose received from the parent.
4. Section 2.4.4, 5th para: Figure 2-9 needs to be explained in more detail.
5. Appendix D.3: It would be useful to have a table summarising the decay chains considered in the hypothetical case, the deterministic cases and the probabilistic cases.
6. Appendix G.7: The distance from the deposition hole to the fracture is one of the outputs from the hydrogeological modelling and is therefore different in each case in the probabilistic calculations. It would be useful to have information on this distance as large calculated distances might be one of the reasons that, for many calculations, radionuclides released from the near-field do not reach the biosphere.
7. Appendix G.7: Testing the discretisation by comparing against SR-Can and a single-compartment seems an odd choice. Any errors will arise due to numerical dispersion, which will probably be driven by the relative size of the largest compartment. Using a growing compartment size for advective transport may not be best – simply using 20 (say) compartments of equal size in all cases might have been better.

Other Observations

1. Section 2.1, 3rd para: SKB refer to the three transport parameters that are calculated by the DFN code and passed on to the radionuclide transport calculations (t_w, Q_{eq} and F) but state that the definition of these is given in Joyce (2010). It would have been helpful if TR-10-50, which refers to these parameters on numerous equations, had included text to explain the definition of these parameters to the reader.
2. Section 2.2.1: This section comprises one sentence and one figure. It should have been extended to provide more context and more explanation. Although it is note stated in the text or the figure, the reviewers assume that Figure 2-4 show groundwater composition in the repository.
3. Section 2.2.2, 1st para: The reviewers would have expected the detail be provided in this report and a summary provided in TR-11-01 rather than the other way around. At least the relevant section number from TR-11-01 should have been provided.
4. Section 2.4.4, 3rd para: This whole paragraph would be better located in Section 2.4.3.
5. Section 3.6, 2nd para: The reviewers consider that the detail should be provided in this report and a summary provided in TR-11-01 rather than the other way around. At least provide the relevant section number from TR-11-01 should be provided.
6. Section 3.6.6: Further confusion is added to the location of parameter values. The text says that some values are defined "here" – presumably meaning this report, but the colloid concentrations are then (in Section 4.5.6) said to come from yet another report.
7. Table 7-1: This is an excellent summary table and one that should have been included in TR-11-01.
8. Figure A-5: the expression for the F-factor for Case #3 is incorrect, although the result is correctly stated.
9. Appendix D.2, 1st para: It should be made clear that the inventory used in the toxicity calculations is the inventory per canister and not the total inventory.
10. Figure D-3: ^{212}Po should read ^{216}Po.
11. Table D-1: Half-life for Pu-240 should be 6.56E3 a.
12. Figure D-7: ^{209}Tl should decay to ^{209}Pb and not ^{209}Bi.
13. Figure D-15: ^{223}Fr should decay to ^{223}Ra and not ^{219}Rn.

TR-10-51

Key Requests for Clarification

1. None.

Other Requests for Clarification

1. Section 3.9.2, 2nd para: SKB should clarify what level of accuracy is considered to "reasonably accurate" with respect to the FARF31code?
2. Section 3.9.2, 2nd para: SKB should justify why the limitation of FARF31 to constant transport properties "poses no problem at the present level of knowledge".
3. Section 3.12.4, 1st para: has a verification document been produced for the Matlab/Simulink version (as opposed to the FORTRAN version) of COMP23?
4. Section 3.20.5, 1st para: the statement that "any groundwater composition (calculated or measured) can be introduced in the tool" goes against the range of conditions given in Section 3.20.2. There is a need to clarify the range of conditions to which Simple Functions can be applied.
5. Section 3.20.5, 2nd para: Is there a danger that the @RISK tool might generate some unrealistic combinations of solubility limits?

Other Observations

1. Section 3.9.2, 2nd para: why mention FARF33 if it is not in fact used?
2. Section 3.20, various paras: Reference is made to Grivé et al. 2010 in the text. Grivé et al. 2010a and 2010b are given in the reference list.
3. Section 3.20.1, 2nd para: replace "confident" with "robust"?
4. Section 3.20.4, 1st para: replace "complete" with "complex"?
5. Section 3.20.4, 2nd and 3rd para: It would have been helpful to provide a brief summary information on how the intercomparison of Simple Functions with PHREEQC and HYDRA-MEDUSA went to save the reader having to refer to Grivé et al. 2010 (be it a or b). It is not enough to say (in 4th para) that Simple Functions is "can be considered to be a good tool for an easy and fast calculation of the solubility of radionuclides" - a statement needs to be provided about its accuracy. A statement that there is "good agreement" is eventually provided in Section 3.20.6 but no reference is given to justify the statement.

TR-10-45 and SKB FEP Database

Key Requests for Clarification

1. None.

Other Requests for Clarification

1. Section 2.1.2: It would be useful if SKB could provide some justification/explanation as to why the near field has nine components, whereas the entire geosphere is considered to be one component, as is the biosphere. Shouldn't there be greater discretisation of the geosphere and biosphere?
2. Section 2.3.4: It is stated that "*input information to the (FEP) database was required only to be made from documents that were dated, signed and provided by the experts assigned for the task".* Was this always the case?
3. Section 3.1.5, Methodology issues: it is stated that "chemical toxicity" FEPs were classified as belonging to the "Biosphere FEPs" category. However, the reviewers can find no evidence of this and question whether chemical toxicity is within the scope of the SR-Site (radiological) safety assessment.
4. Appendix 3: None of the SR-Site initial state FEPs appear to have been checked. Were they checked?

Other Observations

1. Tables 5-2 to 5-7: It is surprising that there is no sub-division of the "radionuclide transport" FEPs (e.g. Ge24 and Ge25) into the individual processes affecting transport (e.g. advection, dispersion, diffusion, rock matrix diffusion, sorption, solubility limitation, decay, ingrowth). It is recognised that some (but not all) of these processes are discussed under specific FEP headings (e.g. Ge12 and Ge13). However, no cross reference is made to these FEPs from the "radionuclide transport" FEPs.
2. Table 5-6: the Section number for FEP Ge25 should be 6.2 and not 3.6.3.
3. Table 5-6: the Section number for FEP Ge25 should be 6.2 and not 3.6.3.
4. Appendices 3 to 10: These appendices provide an audit of SR-Site FEPs against NEA Project FEPs. This results in extensive repetition that is of limited value. It would have been more instructive if the SR-Site FEPs had been audited against the FEPs in the NEA's International FEP database (rather than individual project FEP database).
5. Appendix 6, SR-Site FEP Bu25: "W 2.090 Advection" has an entry of "Advection is considered" but also "Not a relevant FEP".
6. Appendix 7, SR-Site FEP BfT21: "W 2.090 Advection" has an entry of "Advection is considered" but also "Not a relevant FEP".
7. SR-Site FEP F17: In the description field, it is noted that radionuclide transport can occur in gaseous form (C-14, Rn-222 and Kr-85) as well as aqueous form. It is then said that this is handled in SR-Site in COMP23. COMP23 does not consider gases.
8. SR-Site FEP Ge25: This FEP is entitled "Transport of radionuclides in the gas phase". The description/definition is "How radionuclides can be transported by a gas phase". This is not the most illuminating description: the reviewers would have expected some discussion of the key processes to have been given.

TR-10-48

Key Requests for Clarification

1. Section 5.9: What is the basis for the claim that if the uptake of radionuclides is reversible then the impact will likely be negligible whereas irreversible sorption gives a significant potential impact? The basis for this claim is not clear - surely it depends on what fraction of the radionuclides are sorbed onto colloids, not how long they stay on a particular colloidal particle?
2. Section 5.9: Where is the justification given for the rapid reversible sorption/ desorption approach is used in SR-Site?
3. Table 6-1: where, in the suite of SR-Site report, is the potential impact of permafrost and ice sheets on radionuclide transport addressed?
4. Section 6.1.7, Periglacial/glacial climate domains, 2nd para: Is it appropriate to use the pathlines obtained in the groundwater flow simulations for temperate conditions? Might not the permafrost/ice sheet result in different pathlines?
5. Section 6.1.7, Periglacial climate domain, 2nd para: How are Kd values and colloid concentrations chosen to reflect the groundwater conditions of the periglacial/glacial climate domains? Where is this documented?

Other Requests for Clarification

1. Section 6.1.1, 2nd para: The way the RETROCK project is described is rather strange. The text reads as if this project defined how to do radionuclide transport in fractured rock and SKB have then followed that approach. In fact, SKB used this approach well before that and RETROCK was a project that discussed some details. RETROCK made some recommendations, have these been followed up by SKB?
2. Section 6.1.1, 8th para: Can more evidence be cited to show that the potential for transient situations decreases with depth?
3. Table 6-1, groundwater composition: There is a "Yes" in the cell for the process influencing the variable but then the process is described as being not relevant. Should the "Yes" be a "No"?
4. Table 6-1, saturation: There is a "No" in the cell for the variable influencing the process and then the statement "But indirectly, since saturation affects groundwater flow". A clearer explanation needs to be provided as to what is assumed for the purpose of modelling the repository and geosphere.
5. Section 6.1.4, 2nd para: On what basis can it be stated that "the type of processes that typically dominate tracer experiments … are not necessarily of interest on the longer timescales"?
6. Section 6.1.5, 1st para: Explain why "Natural analogue evidence is not directly applicable for the integrated transport model".
7. Section 6.1.5, 2nd para: Are the studies summarised in Miller et al. (1994, 2000) relevant to SR-Site? If so, they should be summarised and their relevance explained; if not, why bother citing the references?
8. Section 6.1.7, Temperate climate domain, 5th para: Why is FARF33 mentioned given that it was not used in SR-Site?

9. Section 6.2.5: Dissolution of gas in shallow groundwaters is explicitly mentioned as a process here (and in Section 5.10.1), so why is there no consideration of it in terms of radionuclide transport?
10. Section 6.2.7, 2nd para: Why are C-14 and Rn-222 the only gaseous radionuclides assessed? H-3, Cl-36, Se-79 and I-129 can all be in gaseous form.

Key Requests for Further Work

1. As noted in Section 2.3.4 of this TN, the potential impact of permafrost and ice sheets on radionuclide transport does not appear to be adequately addressed in the SR-Site reports. SKB should undertake further work to assess issues such as the modification of pathlines, the focussing of discharge into taliks, and the trapping and release (following ice sheet retreat and permafrost melting) of radionuclides below ice sheets/permafrost.

Other Requests for Further Work

1. Section 6.1.4, 1st para: The evidence in the TRUE reports should be summarised so that the reader can confirm that SKB has "an adequate understanding of the relevant processes".

Other Observations

1. Section 1.4: Rather than requiring the reader to read the relevant SR-Can documentation, it would be useful to provide summary of how the list of geosphere variables has been derived. At the very least, the relevant section numbers from the SR-Can documentation should have been provided.
2. Table 1-4: Heat transport from canisters (Ge1) is explicitly identified, however its impact on radionuclide transport is not taken into account in Chapter 6.
3. Table 1-4: Need to explain why gas flow/dissolution (Ge4) is not considered. The reviewers assume that it is due to the fact that gas flow through the geosphere is not explicitly modelled. Instead it is conservatively assumed that gas released from a capsule is released directly into the biosphere.
4. Section 5.9: The "Colloid Transport Project" is mentioned several times with various references to specific journal papers but none appear to describe the project as a whole. The reviewers assume that this relates to work at Äspö. It would have been useful if a full description of the project could be provided.
5. Section 6.1.1, 1st para: Ingrowth should have been explicitly mentioned as a process that influences the transport of radionuclides in the water phase.
6. Section 6.1.1, 1st para: Diffusion (as opposed to matrix diffusion) is mentioned as a process that influences the transport of radionuclides in the water phase. However, it is not mentioned again in Section 6.1 and no justification is given for the exclusion of diffusion along fractures from the radionuclide transport models.
7. Table 6-1, temperature in bedrock: The text relating to "temperature in bedrock" implies that sorption coefficients and matrix diffusivities are

modelled as temperature dependent, whereas the data provided in TR-10-52 clearly are not.

8. Section 6.2.4, 3rd para: It would have been helpful to the reader if the findings of Hartley et al. (2006a) with respect to the capacity for gas migration through the fractured rock at Forsmark were summarised.
9. Section 6.2.8, 3rd and 4th para: It is stated that cautious scoping calculations show insignificant hazards/radiological impacts from the gas release pathway. However, as discussed in Section 2.3.1 of this TN, there are errors in the calculations and non-conservative assumptions are adopted. The correction of these errors and the adoption of more-conservative assumptions results in the risk limit being exceeded.

TR-10-52

Key Requests for Clarification

1. Section 5.3.7, p 171, 5th para: Text states that the large uncertainty ranges in Kd should not give rise to non-conservatism in probabilistic modelling, "as it is the lower tail of the Kd distribution that affects assessment results". This statement is unclear. If the upper estimates of Kd are higher than experimentally observed, presumably they give rise to greater nuclide retardation and hence reduced risk? How is it that the "lower tail of the Kd distribution" is more important?
2. Section 6.7 and 6.8: It is surprising that there is no attempt to justify the parameter choices through any site-specific observations. Are there any site data which could be used to validate transport properties?
3. Section 6.7: Were the various DFN models intended to cover uncertainty for both flow and transport behaviour? Is it possible to specify alternative (more conservative) conceptual models consistent with the available data that would give higher radiological consequences?

Other Requests for Clarification

1. Section 5.3: How is potentially diffusion-dominated transport in the tunnels handled?
2. Section 5.3.2, correlations used in SR-Can modelling: What is meant by saying that the correlations in SR-Can generally agree with those in SR-Site?
3. Section 5.3.2, p 154: The final sentence is unclear. Does it just mean that some species were not in SR-Can?
4. Section 5.3.2, 3rd para: The question of which groundwater to use is discussed. Is the text on page 180 (under Conditions...) intended to address the question raised there? Has it been shown that using SR Site groundwater would not change the conclusions?
5. Section 5.3.5, 5th para. Why is the dry density of backfill in SR Can relevant?
6. Section 5.3.5, p 158, 6th para: Text states that reference groundwaters in Ochs and Talerico (2004) included two alkaline variants, one with pH of up to 13.5. However, without the reviewers obtaining the original source, it is unclear how or why these variants were specified. A pH of 13.5 is very alkaline indeed. Presumably it is a cement porewater? An explanation is needed.
7. Section 5.3.5, p 158, last sentence: On what basis is the claim for 99.9% confidence limits made – is there enough data to support such a claim? In any case, why quote a confidence limit of 99.9%; why not quote 90%, 95% or 100%?
8. Section 5.3.5, p 159, 4th para: Text states that "As the Finnsjön site is located nearby the Forsmark site, and in a broader sense has about the same geological settings, it is suggested to be acceptable to use the Kd data of Ochs and Talerico (2004)". Why are data not available for Forsmark itself?
9. Section 5.3.5, p 160, 1st para: Text states that models need to be used to estimate pore water compositions because there are experimental and conceptual uncertainties in obtaining data directly from compacted bentonite. It is true that there are challenges associated with extracting porewater for analysis. However, it is still valuable to compare analyses of extracted porewater with model results. Was this done?
10. Section 5.3.5, p 161, 9th para: Text states that "Interpolation between the three reference pore water conditions is easily possible for salinity, but

should to be done with care for parameters that are directly linked to others (pH, pCO_2)". What does the term "with care" mean? For parameters that vary non-linearly with mixing, such as pH and pCO_2, linear interpolation should not be used.

11. Section 5.3.5, p 161, last para: Text states that differences in pore water compositions, and hence Kd, between MX-80, Deponit CA-N, and Milos backfill are considered to be negligible "based on the available information". What is this "available information"? A reference should be given.
12. Section 5.3.5, p 162, 1st para: Text states that an increase in temperature to 50°C is expected to lead to a twofold increase of De, while a decrease in temperature to just above freezing is expected to lead to a twofold decrease. What is the basis for this statement? A cross reference to Section 6.8.5 is provided, but this section also does not justify the quoted temperature dependence. At least some published literature seems to suggest a smaller variation, around a factor of 1.5 (e.g. Bastug and Kuyucak, 2005).
13. Section 5.3.7, p 164, 2nd para: Text states that "Recommended De values are based on a regression analysis including all HTO data for Kunigel-V1 and MX-80". Why were the Kunipia-F bentonite data not used? Presumably this was to ensure conservatism, noting that Kunipia-F is almost pure bentonite and hence gives lower De than the other, more impure bentonites?
14. Figure 5-9: Figure gives green lines that bound most of the De data. The caption states that the green lines were placed subjectively. What were the criteria adopted for making these subjective judgements? Several data points plot just outside the delineated fields - why were the green lines not drawn to enclose them too?
15. Section 5.3.7, p 168, 3rd para: Were the Kinipia-F data ignored again when deriving De in order to be conservative?
16. Section 5.3.7, p 170, 4th para: It is stated that the UF-starting Kd is set to ±0.4 log10 units or ±0.6 log10 units, depending respectively upon whether an analogue element shows similar or dissimilar speciation to the element for which Kd is required. What is the justification for these values?
17. Figure 5-12: Figure shows no units for the sum of dissolved chloride and sulphate which are labelled against the x-axis. Presumably molal units are plotted?
18. Section 5.3.7, p 172, 6th bullet: Concerns the Kd values for sulphur and gives a Kd value of 5×10^{-4} m^3/kg for SO_4. The validity of this Kd is questionable. Given that so few data exist and given evidence for weak sorption, it would be more reasonable to recommend conservatively that SO_4 should be treated as non-sorbing. Other programmes have not treated SO_4 as a sorbing. In any case, the buffer material contains trace gypsum, which means that probably SO_4 concentrations will be solubility limited, at least for a substantial period of the buffer's evolution. In this case, it will be invalid to use the Kd approach anyway. So why did SKB not adopt the conservative assumption of no SO_4 sorption?
19. Section 6.7: What evidence is there regarded potential blocking of access to stagnant pore space in fractures (Section 6.7.6 and Appendix A of TR-10-52 seem to assume full accessibility)?
20. Section 6.7: Was a single flow path used for each deposition hole release point (Q1, Q2 and Q3) or were multiple paths per point used?
21. Table 6-81: Why are F_re and F_di so different? What is the meaning of the "Fraction of particles" line?

22. Section 6.7.6: Has the potential for correlation between transport properties and the canisters susceptible to failure been considered or accounted for?
23. Figure 6-71: The agreement between the experimental data and the model looks comparatively poor at early times – does this matter?
24. Section 6.7.8, 4th para: Recharge flow paths are mentioned. In which report are these calculated and discussed in more detail?
25. Section 6.7.10, p 353, 1st para: Is using a 50 m dispersion length within a network of short segments valid? Does MARFA handle this correctly?
26. Section 6.8.4, p 360, (and again on p366 at the end of Section 6.8.6): The idea of limited pore connectivity in the rock matrix is dismissed but no reference is given. What is the evidence for deep penetration? Is the text on p 373 what is intended?
27. Section 6.8.10, p 385: What is the last sentence intended to say? Is there something special about this distribution compared to all the others?
28. Section 6.8.10, p 387: Is the convolution of uncertainty and variability useful – aren't the separate parts needed for different purposes?

Other Observations

1. Table 5.3: Gives the cation exchange capacity (CEC) of MX-80 bentonite as being 85 meq/100 g in the SR-Can assessment, but 75 meq / 100 g in the SR-Site assessment. The preceding paragraph implies that the difference is due to the different densities specified for the bentonite in the two assessments. The reason should have been stated explicitly.
2. Section 5.3.6, p 162, 2nd bullet: Text states that "For Kd, the most significant conceptual uncertainties, *in terms of representing reality*, are related to the description of pore water composition as a function of conditions". It should have also been not that an important source of *conceptual* uncertainty is the validity of Kd concept under certain conditions.
3. Section 5.3.6, p 162, 2nd bullet: The text stating that the composition of pore water composition in compacted bentonite cannot be determined experimentally with any certainty requires qualification. While there are certainly challenges associated with obtaining pore water chemical data, it is feasible to obtain useful information that can be used as a guide to / check on models.
4. Section 5.3.7, p 165, paragraph following Equation 5.4: Text states that "The resulting best estimate De values are 1.4×10^{-10} m^2/s for the buffer ($\rho d = 1{,}562$ kg/m^3) and 1.6×10^{-10} m^2/s for the backfill ($\rho d = 1{,}504$ kg/m^3)". Given that the difference between these values is small compared to the large scatter in the De data shown in Figure 5-6, it is rather strange to recommend different values for the backfill and the buffer.
5. Section 5.3.7, p 167, 1st bullet: Text states that "Accepting the argumentation in Ochs and Talerico (2004), it is suggested that the model prediction by Ochs et al. (2001) for the diffusion of chloride in MX-80 is representative for the range of dry densities considered here". Given that the arguments in Ochs and Talerico (2004) are important, they should have been summarised here.
6. Section 5.3.7, p 167, 1st bullet: Text gives best estimate De values of 1.1×10^{-11} m^2/s for and 1.2×10^{-11} m^2/s for the buffer and backfill respectively. Again, given the fact that the difference between these values is so small compared with the scatter in the data, it is rather strange to recommend different De for the buffer and backfill.

7. Section 5.3.7, p 167, 2nd bullet: Text states that "Upper and lower limits are somewhat subjectively based….". Some indication should have been given of the potential significance for overall uncertainty of the subjective judgements that were made, otherwise this statement is unhelpful to the reader.
8. Section 5.3.7, p 168, 2nd para: Text states that "We refrain from speculating whether this spread [in De] is due to errors (experimental, raw data interpretation, etc.)". The reader is caused to wonder why no speculation is made. It would be better to state simply that the reasons are unknown.
9. Section 5.3.7, p 168, 3rd para: Text gives De for caesium in the buffer and backfill of 4.2 x 10^{-10} m^2/s and 4.8 x 10^{-10} m^2/s respectively. Again, given the uncertainties in De measurements and the fact that these values are quite similar the validity of specifying different De for the buffer and backfill is questionable.
10. Page 168, 1st para sub-section entitled "Diffusion-available porosity" mentions "an explicit effort to distinguish De from ε". However, De is effective diffusivity whereas ε is diffusion-accessible porosity. It would be better to state that an explicit effort was made to distinguish the *effects* of variable De from the *effects* of variable ε.
11. Section 5.3.7, p 168, 4th para; It is stated that published diffusion-available porosities for Cl are a factor of 1.8–3.5 smaller than for HTO. It is then proposed to use a reduction factor of 2.5 based on these data. The fact that the value of 2.5 is only "proposed" again causes the reader to wonder what value was in fact used. This report should clearly specify values for use in the assessment. Additionally, the arithmetic mean of 1.8 and 3.5 is 2.65. Hence, why was a value of 2.5 recommended? While perhaps a minor issue, this case illustrates the inconsistent approaches adopted in this report when recommending parameter values for use in the assessment. In earlier sections, as noted above, the report distinguishes between De values for buffer and backfill, even though the differences between the quoted values for the different materials are smaller than the uncertainties in the data. In contrast, here rounding appears to have been done which seems to cause a relatively large deviation between the actual mean of the data and the recommended value.
12. Section 5.3.7, p 170, 2nd para: Text states that "Based on the available data, the compositions of Deponit CA-N and Milos bentonites are relatively similar to that of MX-80". What is the meaning of "*relatively* similar"? Presumably this statement concerns the mineralogical compositions of the different bentonites (montmorillonite, quartz etc) since they have different exchangeable cation populations. The paragraph continues to state that "Therefore, it can be expected that calculated pore water compositions will be similar, in particular under conditions where carbonate equilibria are controlled by an external pCO_2 (open system)". Given the different exchangeable cations in the different bentonites (dominantly Na in MX-80 and Ca in the others) it would be expected that the pore water compositions would differ to some degree in the different materials.
13. Figure 5-1: Caption should have stated clearly that the coloured circles represent the modelled Da values and reiterate the explanations of RPW, RPWC and HSPW.
14. Section 5.3.7, p 172, 5th bullet: Text references Ochs and Talerico (2004) for details of the selection of UF for Cd and Ni. It is inconsistent with the detailed discussion of other UF in earlier sections simply to reference another literature source without giving details here.

15. Section 5.3.9, p 174, point 9: Text states that the weakly sorbing ion CO_3^{2-} will not correlate. Even accepting that CO_3^{2-} will sorb, the Kd approach is invalid if the specie is solubility-limited, which must be likely given the occurrence of calcite. There should be some discussion of the validity of the Kd concept.
16. Section 5.3.10, p 176, 2nd para: Text states that "The number of significant digits in the Kd values are taken directly from Ochs and Talerico (2004) and does not reflect the accuracy with which the data are estimated". It would have been better to quote a number of significant figures that is commensurate with the precision of the data.
17. Table 5-16: Table gives Kd values. These have been compared with values given for MX-80 bentonite in Bradbury and Baeyens (2002). In the cases of most elements, the values in Bradbury and Baeyens (2002) lie within the ranges quoted in Table 5-16. However, in most cases the ranges in Table 5-16 are wider. The fact that very high upper limits (in comparison with the lower limits and with values in other compilations) are given for many elements in Table 5-16 raises a concern that risk dilution may be a problem in the assessment calculations that use these values.
18. Section 6.7.6: The reasons for the F-factor reduction should have been moved to Appendix A of TR-10-50 since they seem to go beyond the arguments used in that report.
19. Section 6.7.9: Does not mention correlation with failure locations.

Appendix 3: Suggested review topics for SSM

This appendix provides a preliminary list of topics (additional to those already considered) that could be considered in further work by SSM and its external experts. The list has been sub-divided into:

- topics primarily requiring further review (and maybe some limited analysis);
- topics requiring further analysis using mathematical models; and
- topics requiring additional competence.

The list could be extended in light of SKB's responses to the requests for clarification and further work provided in Appendix 2.

Topics Requiring Further Review

1. SKB identified a number of other errors with the radionuclide transport calculations at a late stage in the assessment (see Section 3.7.3 of TR-10-50). Quality assurance checks, undertaken as part of the current review, have identified a number of errors in the documentation of the work undertaken by SKB (see Section 2.5.5 of this TN). In light of this, it is recommended that SSM and its experts should undertake further quality assurance checks, especially for the key calculation cases. Such checks could include auditing the process of managing data sets and the process of passing data between SKB's flow and transport codes.
2. The solubilities of U, Th and Ra have been identified as being of potential importance in affecting the transport of radionuclides (see Section 2.3.2 of this TN). It is recommended that SSM and its experts should undertake a detailed review of SKB's approach to the representation of U, Th and Ra solubilities. Particular issues to address would be: the choice of thermodynamic data; the approach taken to the representation of Ba-Ra co-precipitation; and the importance of the time variation of solubilities on releases from the near field, especially under differing climate conditions. Certain calculations could be undertaken to support the review and its findings.
3. The current review has identified certain issues associated with the treatment of sorption in SR-Site calculations (see Section 2.3.3 of this TN). It is recommended that SSM and its experts should review the Kd values used in SR-Site and evaluate whether they have been used appropriately, given the limitations in the Kd approach (e.g. when Kd has been used, is it always clear that there is no solubility limitation of the element concerned?) and whether the large upper limits given for many elements lead to risk dilution. Certain calculations could be undertaken to support the review and its findings.
4. A number of key parameters affecting risks have been identified (see Section 2.4 of this TN). The following three parameters are beyond the scope of the reviews currently being undertaken by SSM and its experts: the number of failed canisters, the time of canister failure; and the fuel dissolution rate. It is recommended that additional reviews should be undertaken by SSM and its experts to allow SKB's approach to representing these parameters to be critically evaluated. Certain calculations could be undertaken to support the reviews and their findings.

Topics Requiring Further Analysis

1. As noted in Section 2.4 of this TN, it is unclear from TR-10-52 whether the various discrete fracture network models were intended to cover uncertainty for both flow and transport behaviour? It would therefore be useful to investigate whether it is possible to specify alternative (more conservative) discrete fracture network models consistent with the available data that would give higher radiological consequences.
2. TR-10-48 states that the pathlines obtained in the groundwater flow simulations for temperate conditions are used for periglacial and glacial conditions (see Section 2.3.4 of this TN). However, as noted in TR-10-09, "*the flow paths from a repository in a periglacial climate domain will deviate from flow paths developed under present climate conditions*". Therefore, it would be prudent for SSM and its experts to investigate whether pathlines obtained using groundwater flow simulations for temperate conditions are appropriate for use under periglacial and glacial conditions.
3. In Appendix A of TR-10-50, a scoping calculation is presented to demonstrate the effects of channelised flow within an individual fracture on the F-factors used in radionuclide transport calculations can be ignored. There are differences between the two cases presented depending on the F-factor values used within the timescale assessed. Further calculations could be undertaken by SSM and its experts to investigate the impact of representing stagnant water in the discretisation of the far-field model to check the effects of channelised flow by changing the F-factor values and the volume of stagnant water.

Topics Requiring Additional Competence

1. None identified.

Appendix 4: Independent Calculations for F-factor Values

Introduction

Calculations are provided in Appendix A of TR-10-50 to demonstrate the effects of channelised flow within an individual fracture on the F-factors used in radionuclide transport calculations can be ignored. Here some independent calculations are presented to verify these claims. In the following no attempt has been made to justify or check the origins of the governing equations; the emphasis is on ascertaining whether sufficient information is provided in order to reproduce the calculations, and, if so, to verify the reported results.

Independent Calculations

Governing Equations

The SKB calculations consider three separate cases, illustrated in Figure 1. In Case #1 there is no channelling within the fracture and flow is uniform across the whole fracture width. In Case #2 a single channel is considered with flow across 10% of the fracture width – the remainder of the fracture is termed the "stagnant zone". In Case #3 flow is across 10% of the fracture width, divided into 10 separate channels with stagnant zones between them.

The F-factor, or flow-related transport resistance, is used to characterise the transport resistance of the host rock in radionuclide transport calculations. The expression used to calculate the F-factor is

$$F = \frac{2LW_c}{Q} \tag{1}$$

where L is the length of the fracture (m), W_c is the width of the flow channel within the fracture (m) and Q is the volumetric flow rate through the fracture ($m^3\ y^{-1}$).

The cumulative distribution function of the residence time of a non-decaying species in fractures in Laplace space is stated as

$$\tilde{c}_f = \frac{1}{s}\exp\left(-t_w\sqrt{s}\right)\exp\left(-F\left[\psi_m + R_s\psi_s\right]\right) \tag{2}$$

(see Crawford (2008) for derivation). Here s is the Laplace variable (y^{-1}), t_w is the advective travel time (y) and F is the F-factor ($y\ m^{-1}$). ψ_m and ψ_s are fluxes representing diffusion into the matrix and fracture stagnant zone respectively (see below).

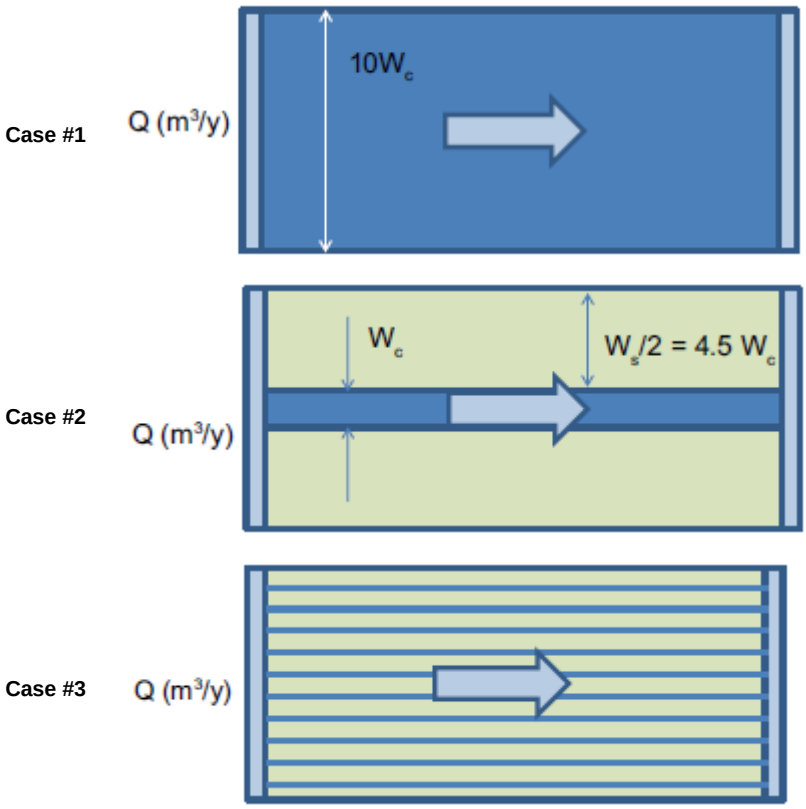

Figure 1: The three fracture flow cases considered (reproduced from TR-10-50 Figures A-2 and A-5).

The surface area ratio, R_s, is defined for a flow channel with symmetrically flanking stagnant zones by

$$R_s = \frac{\delta_s}{W_c} \tag{3}$$

where δ_s is the average transport aperture of the stagnant zone (m) and W_c is the width of the flow channel (m).

The direct matrix flux term ψ_m (m y^{-1}) is given by the expression

$$\psi_m = \sqrt{D_e(\theta_m + K_d \rho_r)s} \tag{4}$$

Where D_e is the effective diffusion coefficient in the rock matrix (m^2 y^{-1}), θ_m is the transport porosity of the rock matrix (-), K_d is the sorption partitioning coefficient of the rock matrix (m^3 kg^{-1}) and ρ_r is the density of the rock matrix (kg m^{-3}).

The indirect matrix flux term via the stagnant zone ψ_s (m y^{-1}) is given by the expression

$$\psi_s = \sqrt{D_w\left(s + \frac{2}{\delta_s}\psi_m\right)}\tanh\left(W_s\sqrt{\frac{1}{D_w}\left(s + \frac{2}{\delta_s}\psi_m\right)}\right) \tag{5}$$

Where D_w is the free component diffusivity in fracture water ($m^2\ y^{-1}$), δ_s is the average transport aperture of the stagnant zone (m) and W_s is the average half width of the stagnant zone (m).

Note that there are conflicting definitions of W_s in the SKB report. In the second paragraph of page 199 it is reported as being the half width of the total stagnant zone, i.e. 4.5 times the width of the flow channel. In Figure A-2 (reproduced here in Figure 1) it is indicated as being the full width of the total stagnant zone, i.e. 9 times the width of the flow channel. It was found that the SKB calculations could only be matched if the former definition is used.

Input Parameters

A list of input parameters and their assumed values is given in Table 2. The source of the value used is also given; not all of the parameter values required were given in Appendix A of TR-10-50, and had to be searched for elsewhere (either in the same report or other reports referenced by it). Thus it is not possible to say for certain that the calculations presented here have been parameterised in exactly the same way as the original SKB calculations.

Table 2: Input parameters used in the calculations

Parameter	Symbol	Value	Source	Comments
Advective Travel Time	t_w	0 s	Pg 201, first paragraph	The advective component is ignored in this study.
F-Factor for Case #1	F_0	5E5 y m^{-1}	Pg 199, final paragraph	Using equation (1), the F-factors for the other cases can be written in terms of F_0.
Effective Diffusion Coefficient of Rock Matrix	D_e	1E-14 $m^2\ s^{-1}$ (3.16E-7 $m^2\ y^{-1}$)	Figure A-3	
Transport Porosity of Rock Matrix	θ_m	2.2E-3	Crawford (2008) pgs 364, 370	Not clear what value was used in the calculations.
Sorption Partitioning Coefficient of Rock Matrix	K_d	0.001 $m^3\ kg^{-1}$	Figure A-3	
Bulk Density of Rock Matrix	ρ_r	2700 kg m^{-3}	Pg 49	Not clear what value was used in the calculations.
Free Component Diffusivity in Fracture Water	D_w	1E-9 $m^2\ s^{-1}$ (3.16E-2 $m^2\ y^{-1}$)	TR-10-52, pg 385	Not clear what value was used in the calculations.
Average transport aperture of the stagnant zone	δ_s	1E-4 m	Pg 199, paragraph 2	The parameter in Figure A-3 is labelled as δ_t but has the same value.
Channel width	W_c	Case 1: 1 m Case 2: 0.1 m Case 3: 0.01 m	Pg 199, paragraph 2; pg 201, paragraph 3	
Average half width of the stagnant zone	W_s	$4.5W_c$	Pg 199, paragraph 2	A conflicting definition is given in Figure A-2.

The use of conflicting units can also lead to confusion. The units used in the governing equations are years, yet many of the parameters (for example, diffusion coefficients) are given in units involving seconds. It would be clearer if a set of base units were employed throughout – where the natural units of a parameter differ from the base units chosen, the value should be given both in the natural and base units.

Results

The expression for the cumulative distribution function of the fracture residence time in Laplace space (equation (2)) was inverted using an implementation of the Talbot algorithm (Talbot, 1979). The results for Cases 1 and 2 (the latter with and without diffusion into the stagnant zone) are shown in Figure 2, along with the original SKB results. There is good agreement between the independent calculations and the SKB results, suggesting that the choice of parameter values not explicitly given in Appendix A were compatible with the original calculations.

Similarly the results for Case #3 (multiple small channels), shown in Figure 3, match those of Case #1 (whole fracture) and therefore are in agreement with the SKB results. Note that the expression for the F-factor for this case, shown in Figure A-5 of TR-10-50 is incorrect, although the result of $0.1F_0$ is correctly stated.

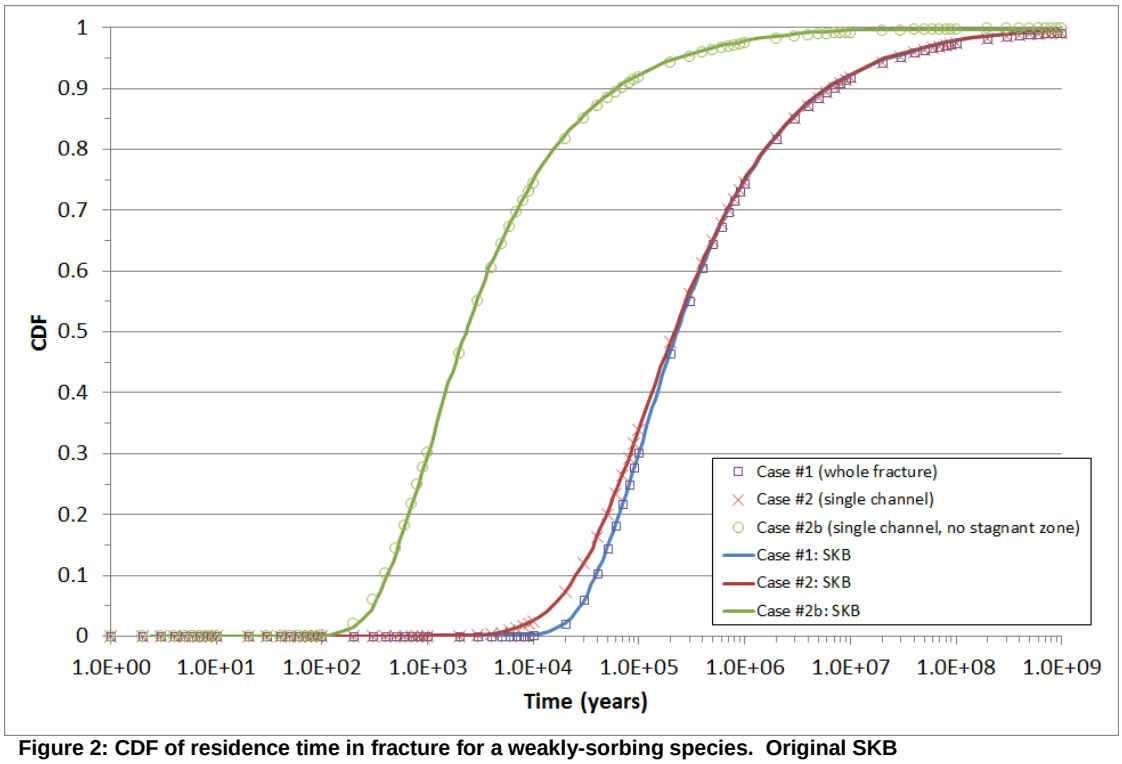

Figure 2: CDF of residence time in fracture for a weakly-sorbing species. Original SKB results shown as lines (data taken from Figure A-3 in TR-10-50), independent calculations as symbols.

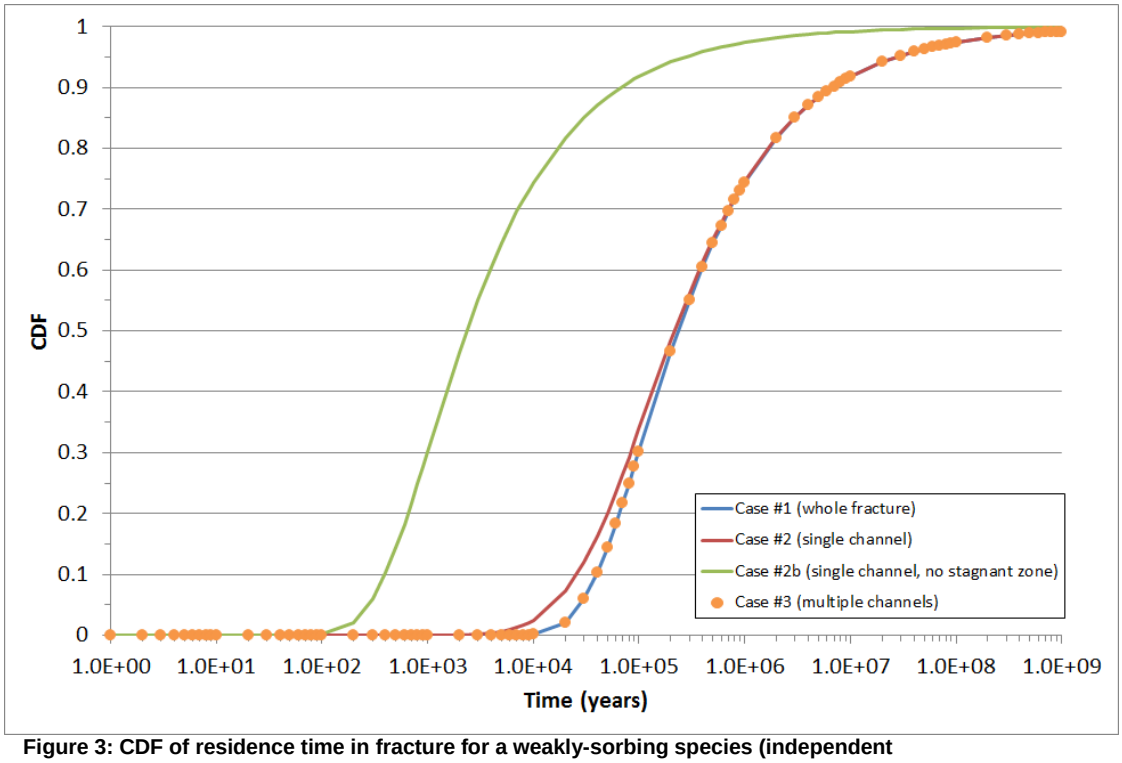

Figure 3: CDF of residence time in fracture for a weakly-sorbing species (independent calculations). Results for multi-channel case are shown as markers.

Next, the effect of varying the base-case F-factor (F_0) on the residence time is examined. Values at each order of magnitude between 10^4 y m^{-1} and 10^7 y m^{-1} were considered; the results of the independent calculations are shown in Figure 4. Here the whole fracture case (Case #1) results are shown as lines, the single channel case with stagnation zone (Case #2) results shown as symbols.

The same parameterisation was used for these calculations as for the previous set, but it was found that the results for Case #2 did not match those reported by SKB (reproduced here in Figure 5). In the independent calculations there is a larger difference between the Case #1 and Case #2 curves, particularly evident for the smaller F-factors. Although not stated in the text, it is possible that another parameter apart from F_0 was altered for these calculations; this parameter would have to play a role in the stagnant zone diffusion term alone since the Case #1 curves match well. This suggestion is supported by the fact that the gap between the Case #1 and #2 curves in Figure A-8 (reproduced as Figure 5) for F_0 = 1E5 y m^{-1} appears to be smaller than that between the same curves for F_0 = 5E5 y m^{-1} shown in Figure A-3 (reproduced here as Figure 2), bucking the trend that the difference between the two cases diminishes as the F-factor increases. The effect is even clearer if Figures A-7 and A-9 are compared.

However, despite this anomaly the independent calculations support SKB's conclusions that the effect of an early breakthrough time promoted by channelling is diminished as the F-factor increases.

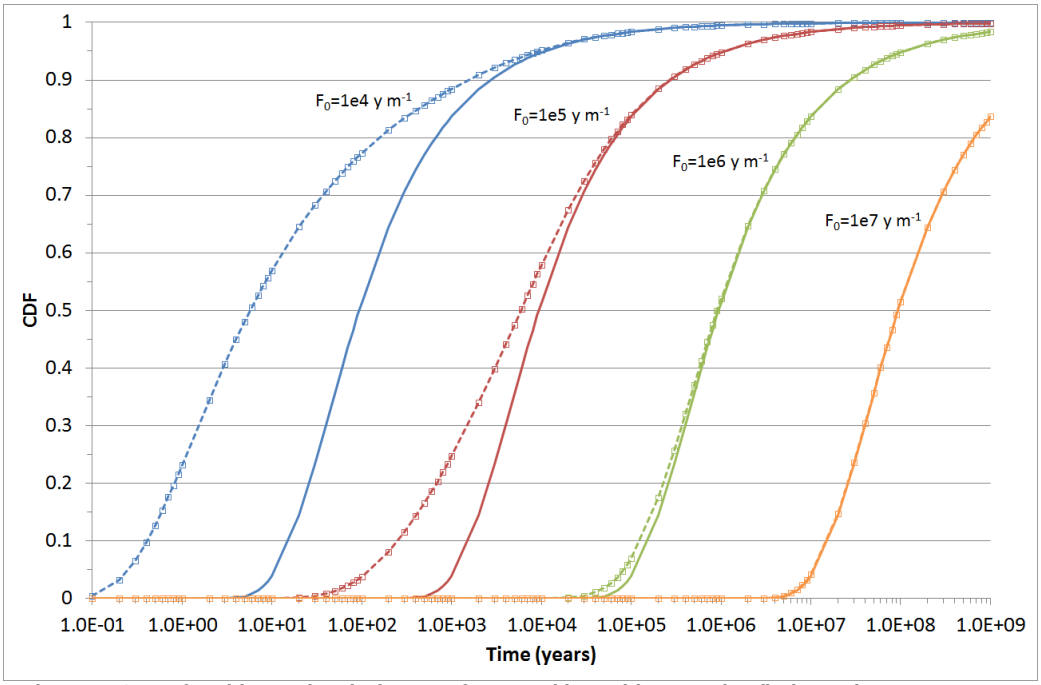

Figure 4: CDF of residence time in fracture for a weakly-sorbing species (independent calculations) showing the effect of varying the base case F-factor on Cases #1 (whole fracture; lines) and #2 (single channel with stagnation zone; symbols).

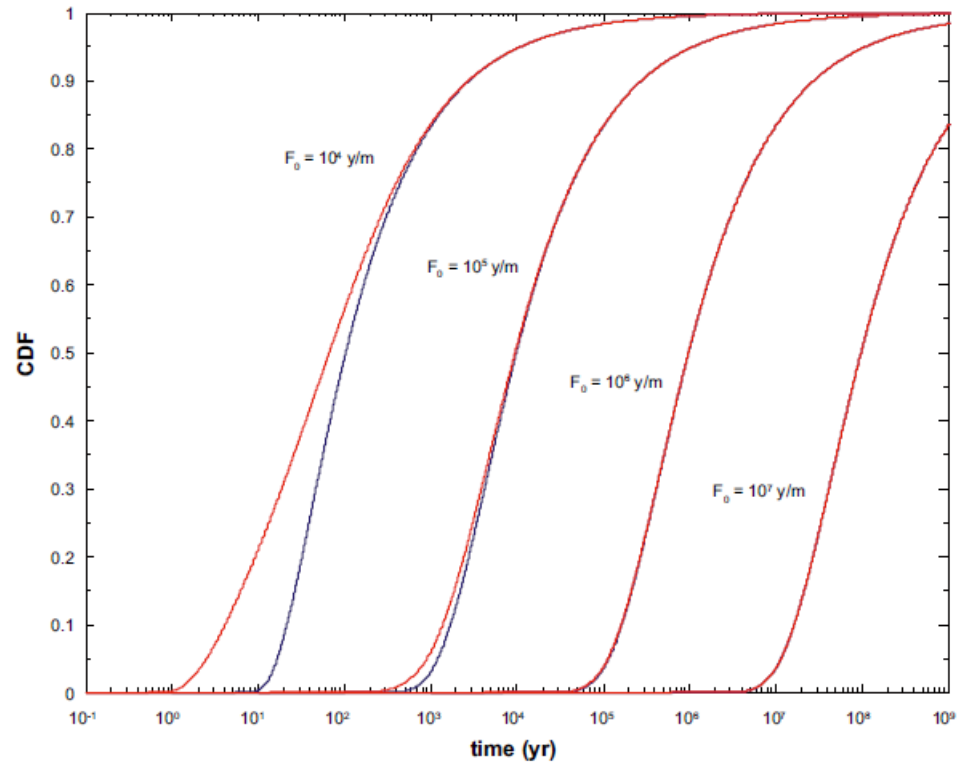

Figure 5: CDF of residence time in fracture for a weakly-sorbing species (original SKB calculations, reproduced from Figure A-8 of TR-10-50) showing the effect of varying the base case F-factor on Cases #1 (whole fracture; blue) and #2 (single channel with stagnation zone; red).

The calculation is repeated for a strongly-sorbing species (K_d = 0.1 m^3 kg^{-1}), with the results of the independent calculations shown in Figure 6. As before, the effect of varying the F-factor is shown on Case #1 (whole fracture) and Case #2 (single channel with stagnation zone). The F-factors used in this calculation are not reported by SKB but are assumed to be the same as for the previous calculation. The results show that channelling causes increasingly early breakthrough times as the F-factor is reduced, but the sorption coefficient has relatively little effect.

The independent calculations were parameterised (except for the Kd and F-factor) in exactly the same manner as the previous calculations, but once again do not match the original SKB calculations shown in Figure A-10 (reproduced here in Figure 7). Without being sure of the input parameters used by SKB, it is impossible to say whether these differences are due to parameterisation or calculation errors, although the former is the more likely.

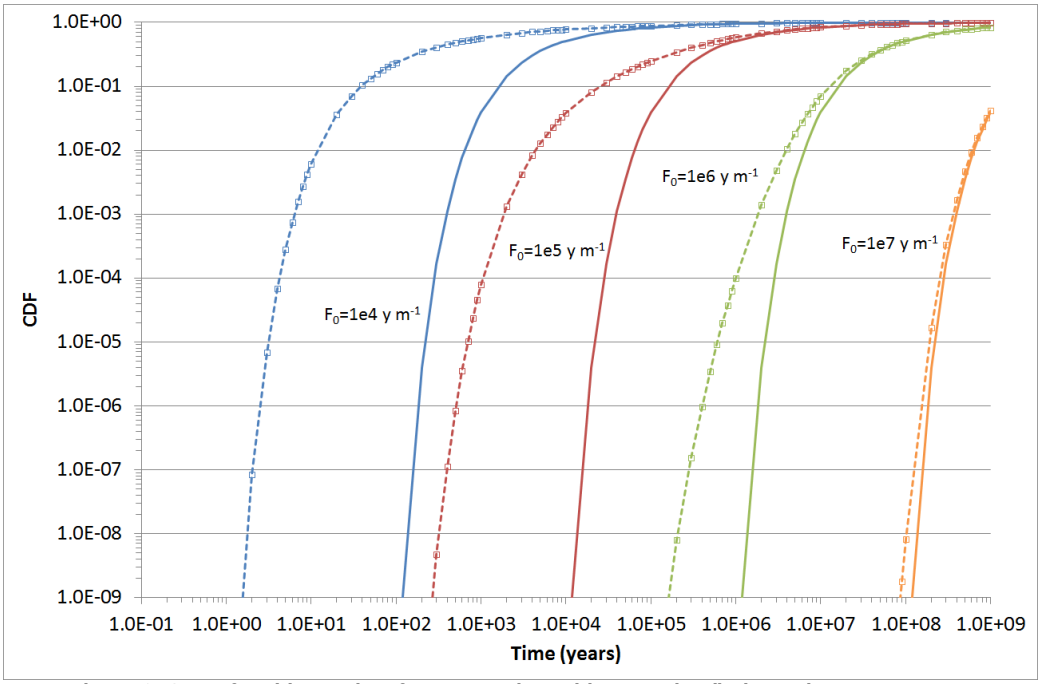

Figure 6: CDF of residence time for a strongly-sorbing species (independent calculations), showing the effect of varying the base case F-factor on Cases #1 (whole fracture; lines) and #2 (single channel with stagnation zone; symbols and dashed lines).

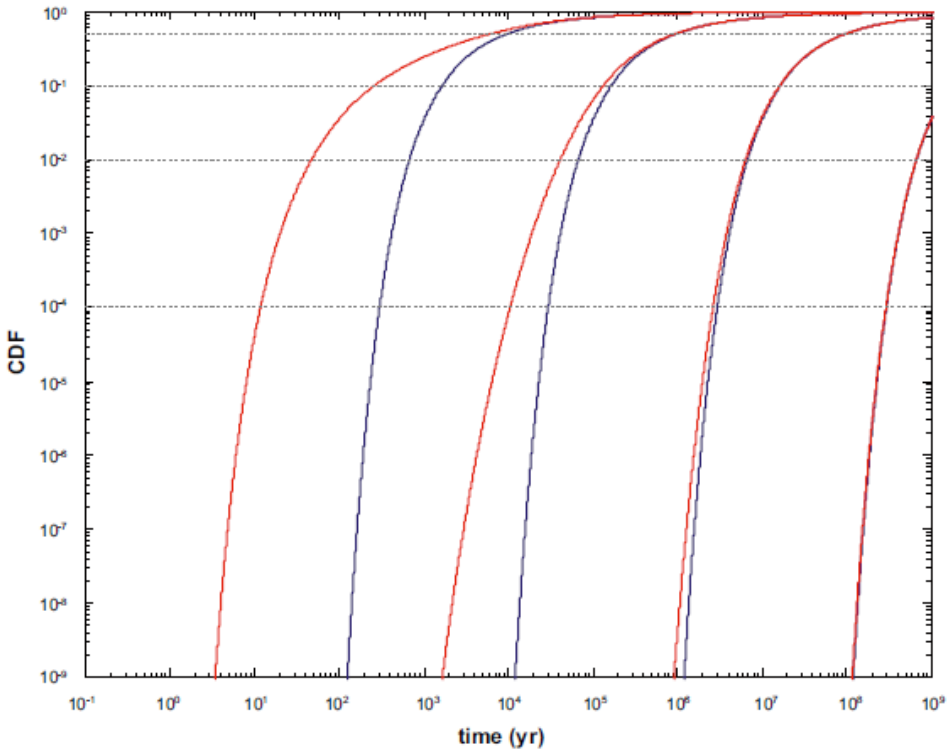

Figure 7: CDF of residence time for a strongly-sorbing species (original SKB calculations, reproduced from Figure A-10 of TR-10-50), showing the effect of varying the base case F-factor on Cases #1 (whole fracture; blue) and #2 (single channel with stagnation zone; red).

Conclusions

Independent calculations have been undertaken to test the claim stated in Appendix A of TR-10-50 that the effects of channelling in fractures can be ignored when choosing F-factor values for radionuclide transport calculations. The independent calculations support the findings of SKB, showing that whilst channelling can lead to earlier breakthrough times, the effect is negligible if flow is through multiple small channels in the fracture (the most likely scenario in real fractures), and diminishes as the base F-factor (calculated by assuming uniform flow through the whole fracture) increases.

Whilst in general the calculations presented by SKB are sound and reasonably well explained, a number of points arose during the undertaking of the independent calculations:

- Not all parameters required for the calculations were given in the Appendix and in some cases it was unclear what values were used in the original calculations.
- A mixture of different units was used, in particular years and seconds.
- In one case conflicting information was given in the text and in figures (the definition of the parameter W_s).
- It was not always clear, when talking about apertures, whether the full or half aperture was meant, or similarly the width of a single stagnant zone or the total width of both symmetrically flanking zones.
- A formula included in an illustration (Figure A-5) was incorrect.

- Using a single set of input parameters it was not possible to match all of the SKB results, but nowhere was the full parameter set given, nor an indication given that it had changed.

References for Appendix

Crawford, J. (2008). Bedrock transport properties Forsmark: Site descriptive modelling. SKB Report R-08-48.

Talbot, A. (1979). The accurate numerical inversion of Laplace transforms. IMA J. Appl. Math. (1979) 23(1): 97-120.

Appendix 5: Independent Calculations for Ra-226 Flux to the Biosphere

Introduction

The relationship between the mobility of thorium around the canister and in the near field and the flux of Ra-226 leaving the geosphere (ultimately linked to the dose) is discussed in a number of places in TR-10-50 (radionuclide transport report). Understanding the origins of the Ra-226 flux to the surface is important, since this radionuclide is one of the main dose contributors.

In Section 4 of TR-10-50, which is concerned with canister failure due to corrosion, it is stated that the inclusion of Th-230 sorption in the near field is considered pessimistic, since this promotes ingrowth of Ra-226 in the buffer. Since Ra-226 is more mobile than Th-230, it is more readily transported through the buffer to the geosphere and consequently to the biosphere. In Section 4.4, it is stated that the release of Ra-226 from the geosphere is almost exclusively due to Ra released from the near field and not to ingrowth in the geosphere (where, for this scenario, rock retention is small since only deposition holes intersected by highly transmissive fractures with high flow rates are considered). In this base case calculation, sorption of Th-230 on the remnants of the buffer material is represented by using a very small solubility limit. The variant calculations reported in Section 4.5.1 of TR-10-50, where thorium sorption in the near field is ignored, support this conclusion because the resultant calculated dose contribution from Ra-226 is lower.

The relationship between the confinement of Th-230 to the near field and the flux of Ra-226 is also discussed in Section 5.2.2 of TR-10-50, which is concerned with failure of the canisters due to shear load in the period between 10^3 and 10^6 years. In this scenario the buffer remains intact but reduced in thickness and the rock retention is considered insignificant due to the large shearing fractures. Ra-226 dominates the dose in the longer term. Here it was found that the solubilities of Th and Ra did not significantly limit the mean release rate of Ra-226. A further calculation (given in Section 5.2.4 of the report) which disregarded both solubility limits and sorption in the buffer indicated that the Ra-226 mean dose was only increased by a factor of two.

Description of Model

Independent calculations have been performed to investigate the relationship between the mobility of thorium in the near field and the flux of Ra-226 to the biosphere. These calculations employ an independent AMBER (Quintessa, 2011) representation of the SKB COMP23 model built for the SR-Can assessment. Full details of the model can be found in Maul et al. (2008), but a summary is presented here for completeness.

The model used considers the pinhole failure mode, which, although considered to be an unlikely scenario, allows the investigation of transport of radionuclides away from the canister through the buffer and geosphere. A single deposition hole is considered, with the main constituents shown in Figure 8. Each of these materials is then divided into a number of compartments. In the original COMP23 model a

number of different pathways were considered; here only the so-called Q1 pathway is included, representing a fracture intersecting the deposition hole. This enables the effect of varying the solubility limit of Th to be clearly seen on the flux of Ra-226 leaving the buffer region and entering the geosphere (which is also included in the model but is not depicted in Figure 8).

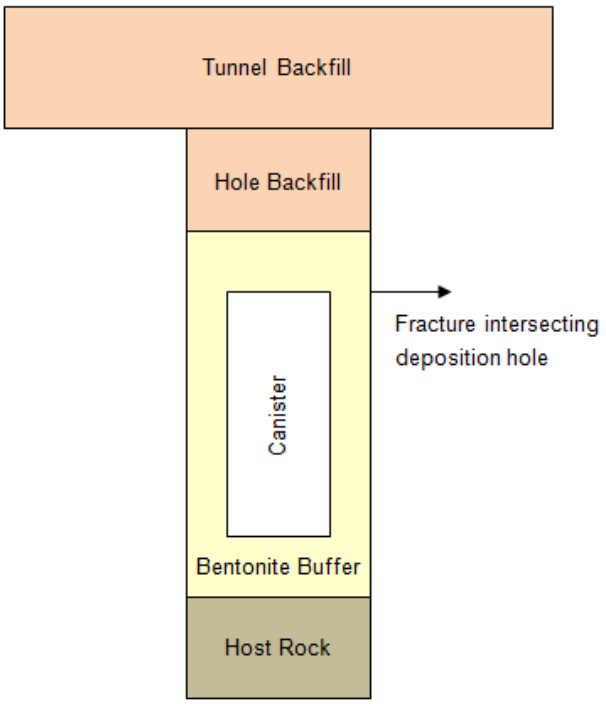

Figure 8: Schematic diagram of the AMBER model used for the independent calculations.

Whilst the original model could be run either in deterministic or probabilistic mode, with all parameters with uncertainty sampled in the latter, here the model is used in probabilistic mode with just the solubility limit of thorium sampled. The solubility limits used in the original probabilistic SKB calculations are correlated and were calculated using PHREEQC and Medusa, using uncertainties in the groundwater speciation to generate a range of values (see SKB (2006) Section 3.4 for details). These values were provided in tabular form by SKB for the review of SR-Can. For the present calculations, in order to obtain a suitable range for the solubility of thorium without sampling for all elements, the minimum, maximum and median of the data previously provided by SKB for Th was taken. This led to a probability density function (PDF) with best estimate 1.47E-3 mol m^{-3} and range [2.96E-5, 2.75E-3] (using a log-uniform distribution).

In order to generate the results presented below, 1000 samples were used.

Results of Independent Calculations

As expected, the independent calculations show that the amount of Th-230 in solution at the pinhole increases with the solubility limit, as demonstrated by the scatter plot shown in Figure 9. This plot also shows that, for solubilities larger than approximately 1E-4 mol m^{-3}, a balance is achieved between the dissolution of

Th-230 and the transport of the radionuclide away from the canister. This threshold point is almost an order of magnitude smaller than the best estimate solubility limit for thorium.

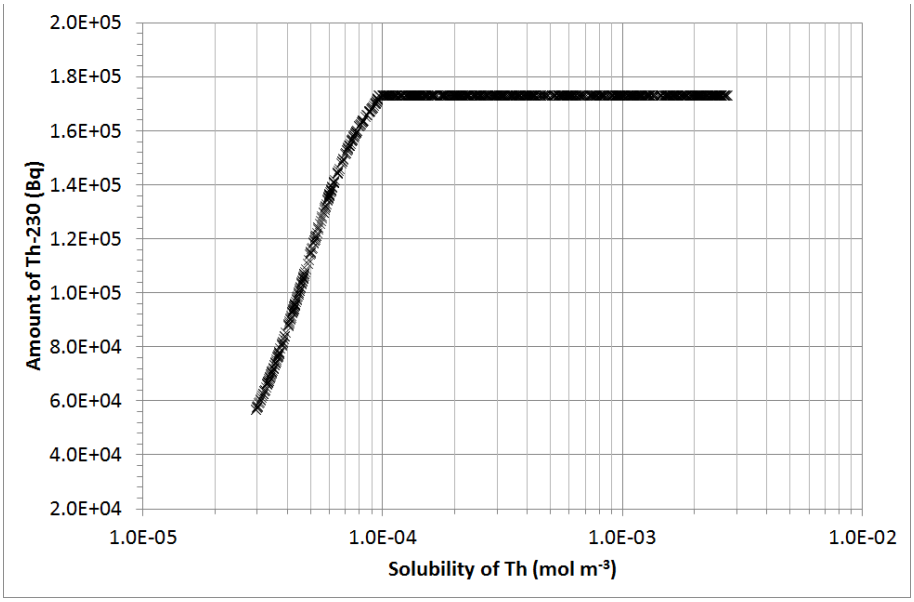

Figure 9: Scatter plot showing how the amount of Th-230 in solution at the pinhole varies with the solubility limit of Th.

The equivalent plot for Ra-226, Figure 10, shows a reverse effect; as the solubility of Th-230 increases and it becomes more mobile, the amount of the more soluble Ra-226 in solution at the pinhole reduces (until the threshold point at which the balance is struck between dissolution and transport).

The evolution of the flux of Ra-226 to the geosphere from the buffer predicted by the model is shown in Figure 11. The 95th, 50th and 5th percentiles are all shown but the 95th and 50th are indistinguishable on this scale. The 5th percentile deviates from the others slightly towards the end of the simulation, indicating that the solubility of Th has a small influence on the flux of Ra-226 leaving the buffer.

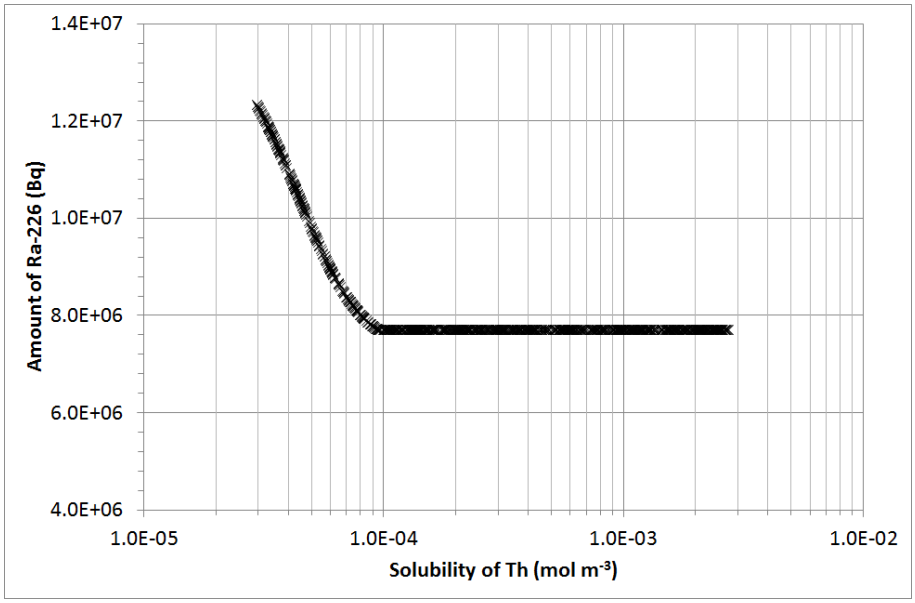

Figure 10: Scatter plot showing how the amount of Ra-226 in solution at the pinhole varies with the solubility limit of Th.

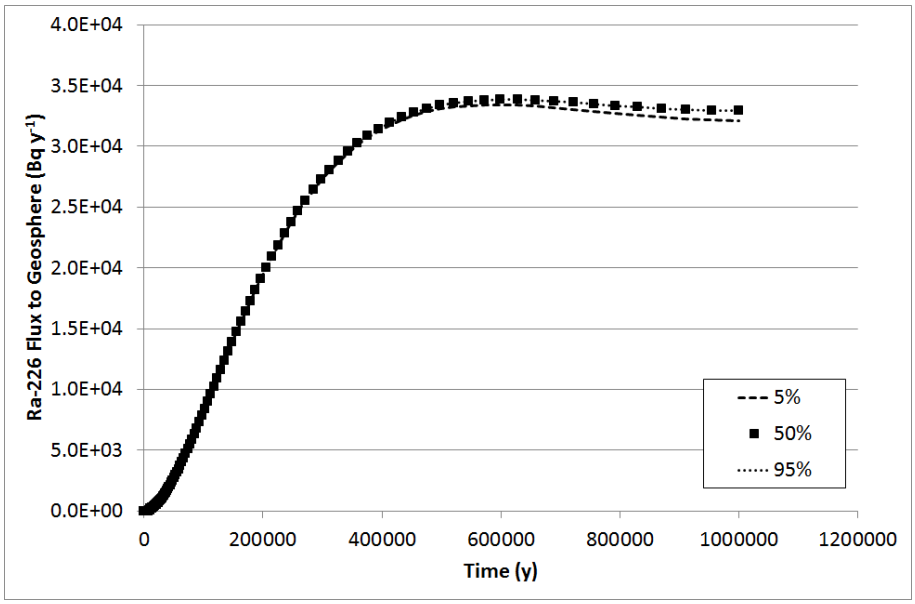

Figure 11: The flux of Ra-226 to the geosphere plotted against time, showing the 5th, 50th and 95th percentiles.

Indeed, a correlation between the solubility limit of Th and the flux of Ra-226 leaving the buffer and entering the geosphere can clearly be seen in Figure 12. However the two parameters are not correlated in the manner that might be expected; a smaller solubility limit and hence immobilisation of Th-230 leads to a reduced flux of Ra-226 at the buffer/geosphere interface, despite the fact that there is more Ra-226 available for transport immediately adjacent to the fuel.

Thus it would appear that the effect of Th-230 immobilisation and ingrowth of Ra-226 near the fuel is insignificant compared to the ingrowth of Ra-226 along the path that the mobile Th-230 takes through the buffer to the geosphere. This is further demonstrated by the fact that a similar correlation can be seen between the flux of Th-230 itself to the geosphere and the solubility limit, as shown in Figure 13. The two effects of immobility of thorium (greater ingrowth of Ra-226 near the canister and reduced flux of Th-230 through the buffer leading to less ingrowth there) work to negate each other, meaning that the overall impact on the flux of Ra-226 is small (Figure 11). Conversely, the overall impact on the flux of Th-230 is larger, as shown in Figure 14.

One would expect that there might be a tipping point at a certain solubility limit where the amount of ingrowing Ra-226 from the immobile Th-230 exceeds that ingrowing from the mobile Th-230 along the transport path. However, this point is clearly some way below the range of solubility limits considered to be relevant and so no further investigation has been made to discover exactly where this may lie. Indeed, the solubility of Th-230 may be of no consequence since the balance between transport and solubility is first struck for values an order of magnitude smaller than the best estimate.

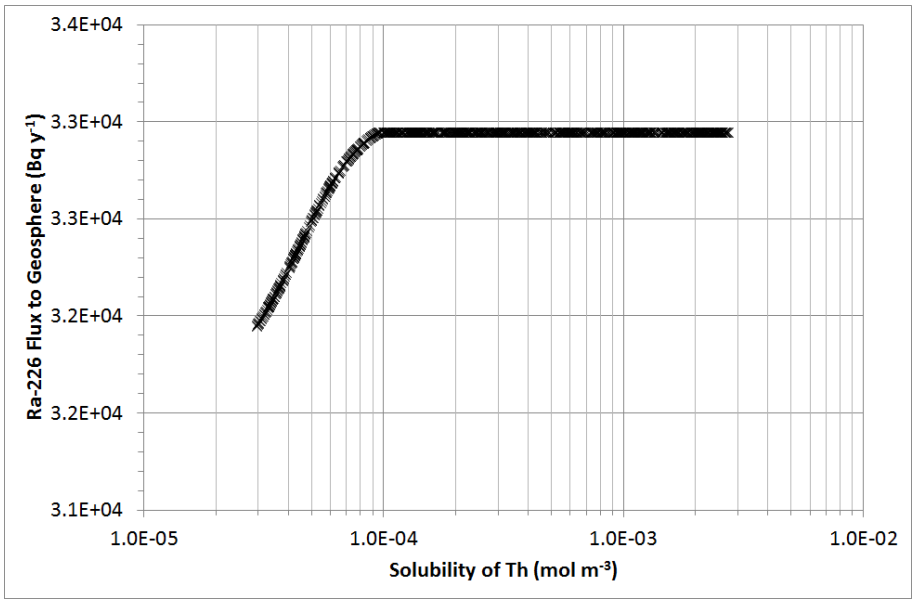

Figure 12: The flux of Ra-226 to the geosphere at 1E6 years plotted against the sampled solubility of Th.

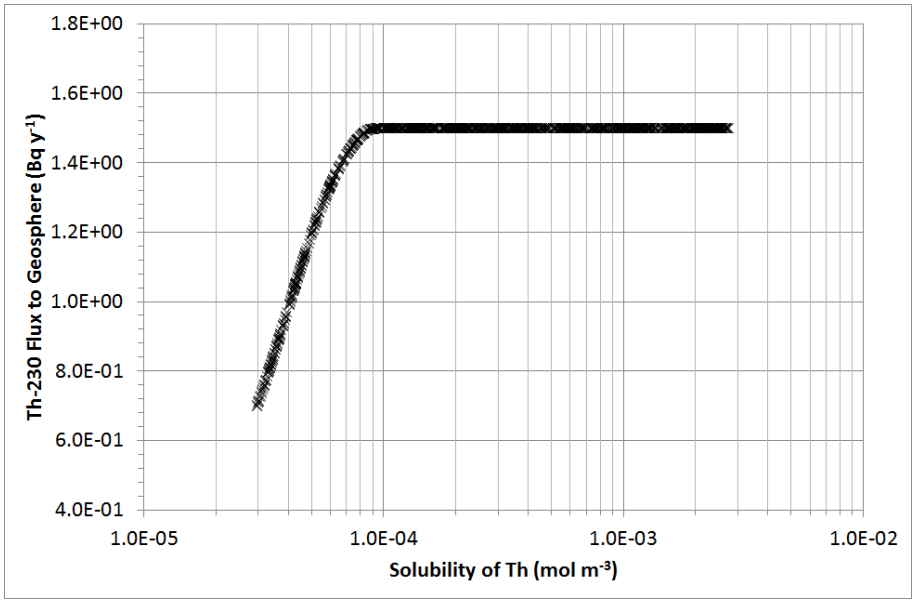

Figure 13: The flux of Th-230 to the geosphere at 1E6 years plotted against the sampled solubility of Th.

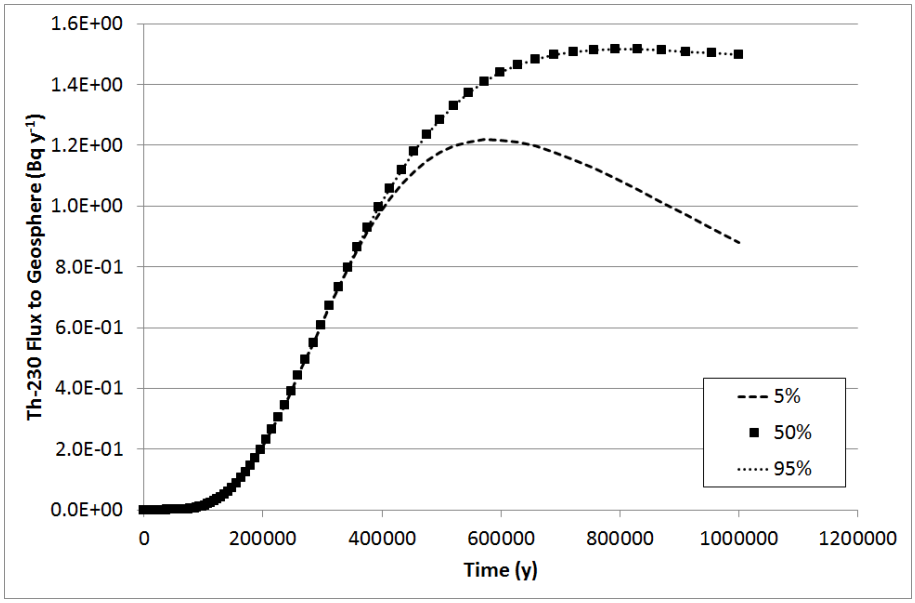

Figure 14: The flux of Th-230 to the geosphere plotted against time, showing the 5th, 50th and 95th percentiles.

The importance of sorption of thorium in the buffer is underlined by considering the extreme cases of no solubility limit (i.e. an essentially infinite limit) and no sorption of thorium in the bentonite. The flux of Ra-226 leaving the geosphere for each of these cases is shown in Figure 15 along with the results from the deterministic base case. If there is no sorption of Th in the buffer, the resultant flux of Ra-226 is over three orders of magnitude larger than the base case over the timescales considered by SKB. Conversely, if the solubility of Th is essentially unlimited but sorption is included in the model, there is little difference between the resultant flux and the base case flux. This is as expected in light of the previous results presented, since

the base case solubility limit already lies in the region where there is a balance between the dissolution of the fuel and diffusion away from the canister.

Also included in the figure are the results from another extreme case, this time with a zero solubility limit for thorium, which has the effect of confining Th-230 to the canister. This results in a very small flux of Ra-226 from the geosphere over the timescales considered, since all the contribution must come Ra-226 ingrowing in the canister and then making its way through the buffer.

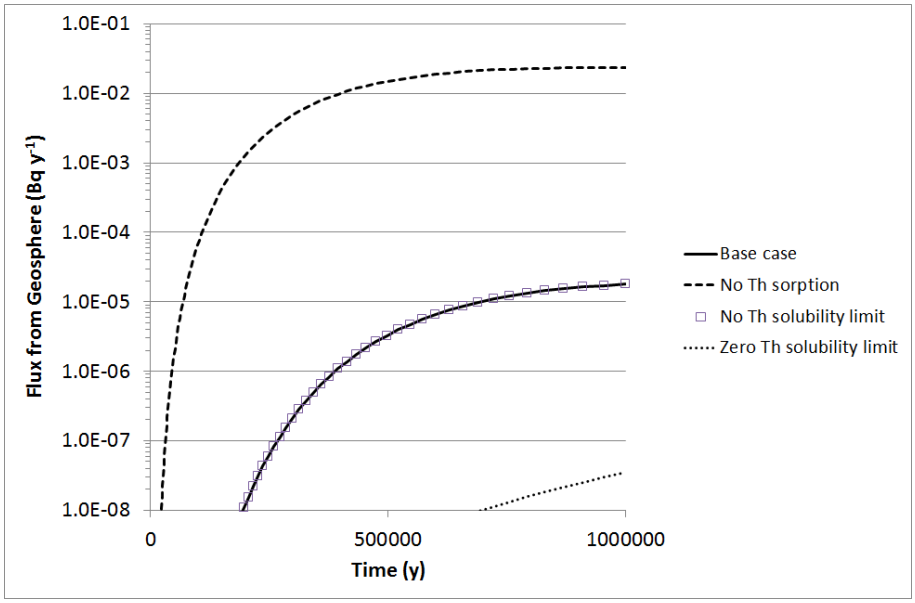

Figure 15: The flux of Ra-226 from the geosphere against time, for the extreme cases of no Th sorption (dashed line); no Th solubility limit (symbols); and a Th solubility limit of 0 mol m^{-3} (dotted line). The base case result is also shown (unbroken line).

Discussion of Results

The results presented are for an intact buffer case, and demonstrate that solubility limits (within the range of suggested values) are not an important constraint on the flux of Ra-226 to the biosphere, but that sorption in the buffer does play an important role.

If the buffer thickness is reduced, as in the shear failure case, then this ability to sorb Th-230 is reduced and the flux of Ra-226 from the geosphere increases accordingly as shown in Figure 16.

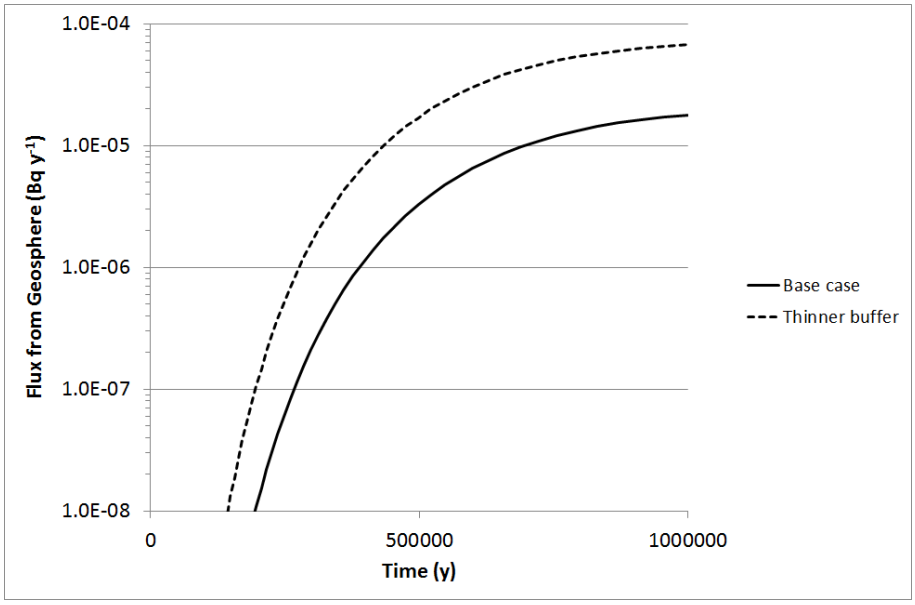

Figure 16: Flux of Ra-226 to the geosphere plotted against time, for the base case and a case with a thinner buffer.

All of this only holds if the movement of Th-230 through the system is reasonably slow, due to the combination of diffusion and sorption. If the buffer is removed and travel times in the geosphere are short, as in the canister corrosion case, Th-230 is moved quickly through the system and has little time to decay to Ra-226, the main dose contributor. Therefore the pessimistic approach taken by SKB of assuming Th-230 is confined to the near field where Ra-226 ingrowth can then occur would seem to be appropriate.

References for Appendix

Maul P, Robinson P, Bond A and Benbow S (2008). Independent Calculations for the SR-Can Assessment: External review contribution in support of SKI's and SSI's review of SR-Can. SKI Report 2008:12.

Quintessa (2011). AMBER 5.5 Reference Guide. Quintessa Report QE-AMBER-3, Version 5.5.

SKB (2006). Data report for the safety assessment SR-Can. SKB Technical Report TR-06-25.

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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 270 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.

Strålsäkerhetsmyndigheten
Swedish Radiation Safety Authority

SE-171 16 Stockholm
Solna strandväg 96

Tel: +46 8 799 40 00
Fax: +46 8 799 40 10

E-mail: registrator@ssm.se
Web: stralsakerhetsmyndigheten.se