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Technical Note 2012:58

Independent radionuclide transport modelling - Reproducing results for main scenarios

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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 utföra oberoende modellering/beräkningar relaterade till transport av radionukliderrelevanta för det planerade KBS-3-förvaret i Forsmark. Grunden för arbetet skall vara SKB: s beräkningsfall som rör kapselbrott till följd av korrosion, kapselbrott till följd av skjuvbelastning och hypotetiska restscenarier som illustrerar barriärfunktioner. SKB:s redovisning av dessa fall ska granskas och ett försök skall göras för att reproducera och/eller kontrollera ett antal beräkningsfall. Detta förväntas ge insikter och kunskaper om SKB:s modelleringsarbete som kan användas för att ge rekommendationer om behov av kompletterande information och förtydliganden som skall levereras av SKB och dessutom ge möjlighet att identifiera kritiska frågor som måste utredas ytterligare inom SSM:s granskning.

Författarnas sammanfattning

Som en del av den inledande tekniska granskningen av SR-Site, tillämpades en förenklad modell för att approximera Svensk Kärnbränslehantering AB (SKB:s) beräkningar när det gäller transport av radionuklider vid det planerade KBS-3-förvaret i Forsmark i Sverige. Målet var att ge insikter och rekommendationer till Strålsäkerhetsmyndigheten (SSM) på förtydliganden och kompletterande upplysningar som skall lämnas av SKB, samt identifiera kritiska frågor som kräver ytterligare undersökning under den följande granskningsfasen på SSM.

Ett mål för detta uppdrag var att bygga en modell för att approximera ett antal beräkningsfall dokumenterade i SKB:s radionuklidtransportrapport inom säkerhetsanalysen SR-Site (SKB, 2010a), nedan kallat "radionuklidtransportrapport." Modelleringen fokuserade på två scenarier: (i) kapselbrott genom korrosion och (ii) kapselbrott genom skjuvbelastning, för att utvärdera om SKB:s beräkningar av utsläpp av radionuklider från brustna kapslar och transporten av radionuklider i grundvattnet till biosfären är lämpliga för att underbygga säkerhetsbedömningen i SR-Site huvudrapport (SKB, 2011).

Granskningen utvärderade (i) transparensen i SKB:s beräkningar (t.ex. är data och beskrivningar tillräckliga för att reproducera beräkningar?), (ii) lämpligheten av SKB:s säkerhetsanalysberäkningar (t.ex. är det några beräkningar som, genom så kallad bias, kan ge upphov till avvikande slutsatser avseende den långsiktiga strålsäkerheten, är förenklingar och antaganden som gjorts för att utföra säkerhetsanalysen lämpliga), och (iii) övergripande beskrivning av SKB:s säkerhetsanalys (t.ex. vilka nyckelfaktorer kontrollerar dosuppskattningar?). Varken tillräcklighet i indata eller lämpligheten hos biosfärsmodellen utvärderades i detta uppdrag.

För vår egenutvecklade modell extraherade vi indata, systembeskrivning och modellantaganden från SKB:s radionuklidtransportrapport (SKB, 2010a) och SKB:s Data Rapport för säkerhetsanalysen SR-Site (SKB, 2010b), nedan kallad "Datarapporten." Resultaten av vår oberoende modell stämde väl överens med SKB resultat. Således drogs slutsatsen från denna inledande granskning att SKB:s beräkningar är transparenta, modellbeskrivningar är tillräckliga, och att data är tämligen kompletta för att en erfaren radionuklidtransport modellerare ska kunna reproducera beräkningarna. SKB: s radionuklidtransportmodeller befanns generellt överensstämma med transportmodeller som används i säkerhetsanalyser utförda av andra nationella organisationer som arbetar med radioaktivt avfall och geologisk slutförvaring.

Inga signifikanta beräkningsproblem identifierades i radionuklidtransportrapporten (SKB, 2010a) som skulle göra SKB slutsatser ogiltiga eller olämpliga. Det bör emellertid poängteras att den oberoende modellutvecklingsstudien och tillhörande granskning som presenterats i denna rapport fokuserar på verifiering av beräkningar, och inte på att utvärdera lämpligheten av data, antaganden och stödjande modeller.

Flera relativt små frågor identifierades med avseende på bristen på klarhet i SKB:s modellbeskrivningar och tillgången på indata. Dessa frågor avser (i) löslighetsgränser för uran (U), radium (Ra), teknetium (Tc) och selen (Se), (ii) ursprungligt innehåll av Se-79, och (iii) sorptionskoefficient (fördelningskoefficient) för plutonium (Pu) i buffertmaterialet. Även om den oberoende utvecklade modellen använde indata från radionuklidtransportrapporten (SKB, 2010a) och Datarapporten (SKB, 2010b), måste några av indatavärdena justeras för att efterlikna SKB:s resultat, även då det inte fanns några uppenbara skillnader i formuleringen och parametreringen mellan de två modellerna.

Dessa skillnader belyser behovet av att SKB tydligt anger vilka indata som används i sina beräkningar och relaterar dessa indata till SKB:s beskrivningar i radionuklidtransportrapporten (SKB, 2010a) och Datarapporten (SKB, 2010b). Till exempel, om SKB har använt en låg löslighetgräns för U i sina beräkningar (under de värden som redovisas i de styrkande tekniska dokument), bör sedan en teknisk grund anges för användning av det låga värdet.

De oberoende beräkningarna kunde inte återge SKB:s resultat som visar minskande trender i radionuklidutsläpp för Th-230 och Ra-226 i skjuvbelastningsscenariot. Därför rekommenderas att SKB förklarar mekanismen som leder till minskande trender och ge delresultat såsom radionukliders flux in i buffertmaterialet, radionuklidkoncentrationer och radionukliders utfällningsmassor i vattnet inuti kapseln för att främja transparensen och stödja SKB:s tekniska grund för nedåtgående trender. Resultaten för SKB: s känslighetsanalys för skjuvbelastningssscenariot befanns i vissa fall vara förvirrande. Till exempel hävdar SKB att förändringar i Ra-lösligheten inte signifikant ändrar dosuppskattningar, trots att SKB identifierat Ra:s löslighet som en viktig parameter i sin känslighetsanalys. Dessutom var det inte tydligt varför SKB associerat ett positivt tecken på känslighetsindex för Th:s löslighet. Ett positivt tecken skulle innebära att användning av ett högt värde för Th:s löslighet bör ge relativt höga dosuppskattningar, men de oberoende verifieringsberäkningarna tycks visa motsatsen (dvs låg Th-löslighet leder till relativt höga Ra-226 utsläpp i närområdet och höga doser).

I de oberoende beräkningarna, befanns dosuppskattningarna för skjuvbelastningsscenariot bero på den förmodade höjden för buffertmaterialblocket i modellen. Om det också är så att SKB:s beräkningar är beroende av denna parameter, kan SKB behöva utveckla en teknisk grund för att motivera valet av buffertblockets höjd i SKB: modellen.

Den tekniska granskningen konstaterade vidare att SKB inte tar hänsyn till gasfasutsläpp av Rn-222 från icke-nedbrutna avfallsformer efter ett kapselbrott. Sådan Rn-222 skulle sönderfalla efter några dagar till Pb-210, som potentiellt bidrar till koncentrationen av Pb-210 i närområdets grundvatten utöver det Pb-210 som redan spårats i SKB:s radionuklidutsläppsberäkningar. Om Pb-210 är en viktig bidragare till dos, så bör SKB antingen ge teknisk grund för att inte räkna med denna extra källa av Pb-210, annars inkludera denna källa av Pb-210 i sin säkerhetsanalys.

När det gäller ytterligare analyser och granskningsinsats av SSM och konsulter, rekommenderar vi att den följande huvudgranskningsfasen bör fokusera på (i) kontroll av antalet kapslar som skulle kunna gå sönder och (ii) en osäkerhetsanalys av tidpunkterna för när kapslar korroderar sönder eller skjuvas sönder av seismiska händelser.

Referenser

SKB. "Long-term safety for the final repository for spent nuclear fuel at Forsmark: main report of the SR-Site project." TR-11-01, Vol. 1-3. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2011.

SKB. "Radionuclide transport report for the safety assessment SR-Site." TR-10-50. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2010a.

SKB. "Data report for the safety assessment SR-Site." SKB TR-10-52. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2010b.

Projektinformation

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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 perform independent modelling/calculations related to the transport of radionuclides relevant for the planned KBS-3 repository at the Forsmark site. The basis for the work shall be SKB's calculation cases related to canister failure due to corrosion, canister failure due to shear-load and hypothetical residual scenarios to illustrate barrier functions. SKB's reporting of these cases shall be reviewed and an attempt shall be made to reproduce and/or check a sub-set of the calculation cases. This is expected to provide insights and knowledge about SKB modelling work that can be used to provide recommendations regarding identified needs for complementary information and clarifications to be delivered by SKB as well as critical issues which need to be further examined.

Summary by the authors

As part of the initial technical review of SR-Site, we applied a simplified model to approximate Swedish Nuclear Fuel and Waste Management Company (SKB) computations related to the transport of radionuclides at the planned KBS–3 repository at the Forsmark site in Sweden. The objective was to provide insights and recommendations to the Swedish Radiation Safety Authority (SSM) on potential clarifications and complementary information to be supplied by SKB, and identify critical topics requiring further examination during the detailed review phase.

The specific objective of this task was to build a model to approximate a subset of calculation cases documented in the SKB Radionuclide Transport Report for the Safety Assessment SR-Site (SKB, 2010a), hereafter referred to simply as the "Radionuclide Transport Report." The modelling focused on two scenarios: (i) Canister Failure by Corrosion and (ii) Canister Failure by Shear Load, to evaluate whether SKB computations of releases of radionuclides from breached canisters and the transport of these radionuclides in the groundwater to the biosphere are appropriate to support the safety assessment documented in the SR-Site main report (SKB, 2011). The review evaluated (i) transparency of the SKB computations (e.g., are data and descriptions sufficient to reproduce computations?), (ii) appropriateness of the SKB performance assessment computations (e.g., are there any computations that could bias safety conclusions; are simplifications and assumptions made for the performance assessment appropriate?), and (iii) description of the overall SKB performance assessment (e.g., what key fac-

tors control dose estimates?). Neither adequacy of the input data nor the adequacy of the biosphere model was evaluated in this task.

For our independently developed model, we extracted input data, system description, and model assumptions, from the SKB Radionuclide Transport Report (SKB, 2010a) and the SKB Data Report for the Safety Assessment SR-Site (SKB, 2010b), hereafter referred to simply as the "Data Report." The results of our independent model compared well with SKB results. Therefore, this initial review concluded that computations by SKB are transparent, model descriptions are adequate, and the data are reasonably complete to allow an experienced radionuclide transport modeller to reproduce computations. SKB's radionuclide transport models were found to be generally consistent with transport models used in performance assessments conducted by other national organizations working in radioactive waste management and geological disposal. No significant computational issues were identified in the Radionuclide Transport Report (SKB, 2010a) that would render SKB conclusions invalid or inappropriate. It should be kept in mind, however, that the independent model development study and the associated review activities focused on verifying computations, and not on evaluating the adequacy of data, assumptions, and supporting models.

Several relatively minor issues were identified with respect to lack of clarity in the SKB model descriptions and availability of input data. These issues relate to (i) solubility limits for uranium (U), radium (Ra), technetium (Tc), and selenium (Se); (ii) initial inventory of Se-79; and (iii) sorption coefficient (distribution coefficient) for plutonium (Pu) in the buffer material. Although the independently developed model adopted input data from the Radionuclide Transport Report (SKB, 2010a) and the Data Report (SKB, 2010b), some of the input data values had to be adjusted to emulate the SKB results, even where there were no apparent differences in the formulation and parameterization between the two models. These discrepancies highlight a need for SKB to unequivocally specify data used in its computations and to compare such input data to SKB descriptions in the Radionuclide Transport Report (SKB, 2010a) and the Data Report (SKB, 2010b). For example, if SKB has used a low U solubility limit in its calculations (below the values reported in the supporting technical documents), then a technical basis should be provided for the use of the low value.

The independent computations were unable to reproduce the SKB results showing decreasing trends in radionuclide releases for Th-230 and Ra-226 in the Shear Load Failure scenario. Therefore, we recommend that SKB explain the mechanism that leads to the decreasing trends and provide intermediate results such as radionuclide release rates into the buffer material, radionuclide concentrations, and precipitated radionuclide masses in the water inside the canister to promote transparency and to support the SKB technical basis for the decreasing trends.

The SKB sensitivity analysis results for the Shear Load Failure scenario were found to be confusing in some cases. For example, SKB argues that changing the Ra solubility does not significantly change dose estimates, although SKB identified Ra solubility as a key parameter in the SKB sensitivity analysis. Also, it was not clear why SKB has associated a positive sign in the sensitivity index for Th solubility. A positive sign would imply that using a high Th solubility value should produce relatively high dose estimates, yet the independent verification computations appear to suggest the opposite (i.e., low Th solubility leads to relatively high Ra-226 near-field releases and high doses).

In the independent computations, the dose estimates for the Shear Load Failure scenario were found to depend on the assumed height of the buffer material block in the model. If it is also the case that SKB computations depend on this parameter, then SKB may need to develop a technical basis for justifying the selection of buffer block height in the SKB model.

The technical review noted that SKB did not account for Rn-222 release as a gas phase from non-degraded waste forms after a canister breach. Such Rn-222 would decay after a few days to Pb-210, potentially contributing to the concentration of Pb-210 in the near-field groundwater in addition to the Pb-210 already tracked in the SKB radionuclide release computations. If Pb-210 is a significant contributor to dose, then SKB should either provide a technical basis for not accounting for this additional source of Pb-210, or else include this source of Pb-210 in its performance assessment.

With regards to additional analyses and review effort by SSM and consultants, we recommend that the detailed review phase should focus on (i) verification of the number of canisters that could be breached and (ii) the timing of breach by corrosion and by damage initiated by seismic events, while also accounting for uncertainties and variability.

References

SKB. "Long-term safety for the final repository for spent nuclear fuel at Forsmark: main report of the SR-Site project." TR-11-01, Vol. 1-3. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2011.

SKB. "Radionuclide transport report for the safety assessment SR-Site." TR-10-50. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2010a.

SKB. "Data report for the safety assessment SR-Site." SKB TR-10-52. Stockholm, Sweden: Svenska Kärnbränslehantering AB. 2010b.

Project information

Contact person at SSM: Shulan Xu Framework agreement number: SSM2011-4243 Call-off request number: SSM2012-142 Activity number: 3030007-4030



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Technical Note 33 2012:58 Independent radionuclide transport modelling – Reproducing results for main scenarios

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Content

1. Introduction	3
2. General model description	3
3. Canister failure by corrosion scenario	5
3.1. Model setup and assumptions	5
3.2. Results and discussion	8
4. Scenario for canister failure by shear load	.19
4.1. Model setup and assumptions	.19
4.2. Results and discussion	.25
5. Conclusions	.33
6. References	.34
Appendix 1: Coverage of SKB reports	.35
Appendix 2: Suggested needs for complementary information from	
SKB	.36
Appendix 3: Suggested review topics for SSM	.39

1. Introduction

This technical note documents results from a relatively simple model developed by the reviewers at the Center for Nuclear Waste Regulatory Analyses (CNWRA[®]), Southwest Research Institute[®] (SwRI[®]). The objective of this exercise was to check whether the Swedish Nuclear Fuel and Waste Management Company (SKB) computations documented in SKB's Radionuclide Transport Report for the Safety Assessment SR-Site (SKB, 2010a) for scenarios related to canister failure by corrosion and canister failure by shear load, could be replicated and thereby evaluate whether the SKB radionuclide transport computations are appropriate to support the conclusions in the SR-Site main report (SKB, 2011). The review focused on a selected set of computations for two key scenarios-Canister Failure by Corrosion and Canister Failure by Shear Load. The review evaluated the transparency of the SKB modelling (e.g., are data and descriptions sufficient to reproduce computations?), appropriateness of the performance assessment computations (e.g., are there any computations that could bias safety conclusions; are simplifications and assumptions appropriate for a performance assessment?), and effectiveness of the description of the overall SKB performance assessment (e.g., what factors control dose estimates?). Adequacy of the input data was not evaluated in this review. For example, it was noted that the waste form degradation rate plays a major role in the dose estimates, but the adequacy of the range of SKB input values for the waste form degradation rate was not evaluated in this review. Also, the SKB biosphere model, another important component of the SKB performance assessment that merits a detailed review, was not evaluated as part of this assignment.

The complete citations for all of the SKB documents consulted for this review, with comments about how the documents were used, are provided in Appendix 1. Two SKB reports and accompanying appendices—TR-10–50, Radionuclide Transport Report for the Safety Assessment SR-Site (SKB, 2010a), hereafter referred to simply as the "Radionuclide Transport Report;" and TR-10–52, Data Report for the Safety Assessment SR-Site (SKB, 2010b), hereafter referred to simply as the "Data Report,"—are without exception the source of all of the data in our verification computations. Only a few equations are provided in this report to clarify the computational approach and meaning of parameters, the remaining approaches and algorithms are described in words instead, to reach a balance between description detail and report readability. The reviewers have adopted first-person usage in this technical note to make a clear distinction between our verification computations and the SKB computations. For example, we use terms such as "we computed" or "our computations" to clarify which modelling tasks have been performed as part of this review assignment as opposed to the modelling that was performed by SKB.

2. General model description

Based on descriptions SKB provided in the Radionuclide Transport Report, the following model components were implemented in our verification model using GoldSim (GoldSim Technology Group, LLC, 2012): (i) waste form (as a source term), (ii) water volume inside the canister (as a uniform mixing cell), (iii) the buffer material (as a diffusive barrier), and (iv) an advective-dispersive transport pathway (to represent radionuclide transport in the geosphere). The biosphere system was not explicitly modelled. Instead, landscape dose factors (LDF) and pulse LDF for temperate conditions were used to convert radionuclide release rates in units of activity/time into release rates in units of dose per year. To limit the input data

needs for the verification task, only a small set of radionuclides (i.e., 19 compared to SKB's 37) was considered, including fission and activation products as well as decay chains. The radionuclides considered in our verification computations are

C-14, Cs-135, I-129, Nb-94, Ni-59, Np-237, Pb-210, Pu-239, Pu-240, Pu-242, Ra-226, Se-79, Tc-99, Th-230, U-233, U-234, U235, U-236, U-238

The following decay chains were considered

 $\begin{array}{l} Np\text{-}237 \rightarrow U\text{-}233\\ Pu\text{-}239 \rightarrow U\text{-}235\\ Pu\text{-}240 \rightarrow U\text{-}236\\ Pu\text{-}242 \rightarrow U\text{-}238 \rightarrow U\text{-}234 \rightarrow \text{Th-}230 \rightarrow \text{Ra-}226 \rightarrow \text{Pb-}210 \end{array}$

Initial inventories and half-lives were taken from the Data Report. GoldSim model files include data used in the verification computations and are attached to CNWRA scientific notebook 1135E (Pensado and Mohanty, 2012) as part of our quality assurance records.

Pu-241 and Am-241 were not included directly in our verification computations because these radionuclides are relatively short lived (half-lives of 14.3 and 432.7 years, respectively). However, SKB did explicitly model Pu-241 and Am-241. Both decay into Np-237 and contribute significantly to the Np-237 inventory. Thus, for the simplified computations, we assumed that the initial inventories of Pu-241 and Am-241 had already fully decayed into Np-237, and we added this total to the initial inventory of Np-237. Consequently, the initial Np-237 inventory in the verification computations was 22.85 tons (for 6,103 canisters), which is 3.34 times the Np-237 inventory in Table 3-3 of the Data Report (i.e., the Np-237 activity of 1.78×10^{14} Bq in Table 3-3 of the Data Report is equivalent to 6.83 tons).

With few exceptions, the verification computations used deterministic values and distribution functions for input parameters that were taken from the Radionuclide Transport Report. The few exceptions were related to distribution functions for corrosion release fractions. SKB proposed the use of double-triangular distributions, constructed as two opposing right-angle triangles, with the area of each triangle enclosing 50 percent of the probability. Given that such a distribution type is not directly available in GoldSim, standard triangular distributions were used instead. The triangular distributions were selected to be symmetric around the mode (i.e., such that the mode equals the median of the distribution), with the median or mode matching the median of the SKB distributions. One end of the distribution had to be adjusted to match the SKB median value. The selection of triangular distributions would yield comparable results to SKB results in the verification of stochastic computations. In principle, any distribution can be specified in GoldSim by the use of cumulative distribution functions through look-up tables. For example, we employed user-defined cumulative distribution functions to specify doubletriangular distributions for instant release fractions, but it required some effort to compute a collection of quantiles and manually input those quantiles into a GoldSim model file.

Temperate LDF for continuous releases, taken from Table 7-13 of the Data Report, were directly used to transform far-field releases in units of Bq/yr into doses in units of Sv/yr. Pulse LDF values from Table 7-14 of the Data Report were used to translate instantly released inventories of Cs-135, I-129, Se-79, Tc-99, Ni-59, and

Nb-94, in units of Bq, into doses in units of Sv/yr. We assumed flat pulse doses for a relatively short period (compared to a simulation time of one million years) after failure of the canister. Beyond the "pulse time window," temperate LDF values were used to compute near-field doses per year. The pulse LDF values were only used to compute near-field doses.

Pulse LDF values were not used in the computations of far-field doses in the corrosion failure scenario or for doses in the shear load failure scenario. Instead, temperate LDF were used to translate release rates in units of Bq/yr to doses in units of Sv/yr in the deterministic computations. SKB opted not to include an instantly released fraction (IRF) in the far-field computations in the corrosion failure scenario, with the exception of Tc-99 (Radionuclide Transport Report, page 58). The IRF is the fraction of the inventory released immediately into the in-canister water after canister failure. We agree with the SKB conclusion that pulse releases play a minimal role in the average dose for stochastic runs with random canister failure time, provided that the duration of pulses is small with respect to the simulation time of one million years. For that reason, IRF (and hence, pulse LDF) were disregarded in our computations for the stochastic simulations, (i.e., the IRF was set equal to zero, and continuous LDF values were used). We only used pulse LDF values in the deterministic computations of near-field doses in the corrosion failure scenario.

3. Canister failure by corrosion scenario

In the scenario for canister failure by corrosion, SKB considered that canisters fail by corrosion after the buffer material is eroded away by fast water flows. The onset of erosion and failure of the canister by corrosion is considered by SKB to take significant time, at least one hundred thousand years. At the time radionuclide releases occur, the buffer material would not be a barrier limiting radionuclide release. SKB considers radionuclides to be transported in groundwater flowing in fractured rock and released to the biosphere. In this section, we discuss the use of our simplified model to approximate the SKB computations for the scenario for canister failure by corrosion, and we compare the model results to SKB results.

3.1. Model setup and assumptions

The near-field model elements of the SKB scenario for Canister Failure by Corrosion in the Radionuclide Transport Report are summarized in Figure 1(a). In the verification computations, we assumed the waste form to degrade at a constant rate. The time for complete degradation is sampled from a log-triangular distribution ranging from one million to one hundred million years, with the mid-point of the distribution at ten-million years. Mass balance computations in GoldSim account for decay and ingrowth. We assumed that radionuclides are released into the in-canister water in congruent proportion to the number of atoms in the waste form. Consistent with the SKB description, we considered that a fraction of the inventory (i.e., the IRF) would be instantly released into the in-canister water immediately after canister failure. The following radionuclides have an IRF: C-14, Cs-135, I-129, Se-79, Tc-99, Ni-59, and Nb-94. In addition, a fraction of the radionuclide inventory is present in the cladding and metallic structures, and its release into the in-canister water is controlled by a corrosion rate. This fraction is referred to as corrosion released fraction (CRF). Consistent with the SKB approach, we sampled the time for full depletion by corrosion from a log-triangular





distribution ranging from 100 to 10,000 years, with the distribution mid-point at 1,000 years. The following radionuclides have a CRF: C-14, Se-79, Tc-99, U-233, Ni-59, and Nb-94.

Radionuclides released into the in-canister water (whether by waste form degradation, or as the IRF or CRF) are assumed to be uniformly mixed in a volume of water equal to 1 m³. The sum of the concentrations of the isotopes of a single element such as uranium (e.g., U-233, U-234, U235, U-236, and U-238) is compared to the assumed solubility limited concentration for that element. If the modelled concentration exceeds the solubility limit, the excess mass is assumed to precipitate. Precipitation for each radionuclide is assumed to occur in proportion to the total mass in the system (i.e., mass in solution and mass in the precipitated form). Decay and ingrowth are computed for both the mass in solution and the precipitated mass. If the total concentration of the isotopes in solution drops below the solubility limit, a fraction of the precipitate is allowed to dissolve to maintain the aqueous concentration of the element at the solubility limit.

Radionuclides are released into the far field by advection. Flow rates of the order of $q = 1 \text{ m}^3/\text{yr}$ "wash away" radionuclides from the near field with a release rate computed as $c \times q$, where *c* is the radionuclide concentration in the in-canister water. The flow rate *q* in the SKB computations is relatively high, and so release rates to the far field are only weakly dependent on the magnitude of *q*. The main controlling factors for releases into the far field are initial inventories, waste form degradation rate, and solubility limits. The IRF is associated with spike releases, which are not important for average dose estimates as long as the canister failure time is a random variable that is widely distributed (e.g., spread between 100,000 and

1,000,000 years), the number of canisters failed by corrosion is small, and the duration of the pulse releases is "short" compared to one million years. Figure 1(b) is a summary of the model components for the far-field transport in the geosphere. Geosphere transport of radionuclides takes places in the form of advective-dispersive transport along fractures. Matrix diffusion causes mass exchange between fractures and the rock matrix along a direction perpendicular to the flow direction. In the model, diffusion in the rock matrix along longitudinal direction (i.e., the flow direction) is ignored. Equilibrium linear sorption operates in the rock matrix.

The advective-dispersive equation to compute radionuclide transport through the fracture for radionuclide i is

$$\frac{\partial c_i}{\partial t} = \frac{\alpha L^2}{t_w} \frac{\partial^2 c_i}{\partial x^2} - \frac{L}{t_w} \frac{\partial c_i}{\partial x} - \lambda_i c_i + \lambda_p c_p \frac{M_i}{M_p} + \frac{1}{b} D_i \frac{\partial \bar{c_i}}{\partial z}$$
[1]

and the mass conservation equation in the rock matrix is

$$R_i \frac{\partial \bar{c}_i}{\partial t} = D_i \frac{\partial^2 \bar{c}_i}{\partial z^2} - \lambda_i \bar{c}_i R_i + \lambda_p \bar{c}_p R_p \frac{\theta_p M_i}{\theta_i M_p}$$
[2]

where

Subscript i	— radionuclide <i>i</i>
Subscript p	— parent radionuclide
Ci	— concentration of radionuclide <i>i</i> in the
	fracture water (M/L ³)
α	— dispersivity fraction $= 0.1$
L	— pathway length (L)
t_w	— water travel time (T)
X	— flow direction (L)
λ	— decay rate $(1/T)$
Μ	— molar mass (M/mol)
b	— fracture semi-aperture (L)
Θ_i	— rock matrix porosity accessible to
	radionuclide <i>i</i> (dimensionless)
Θ_p	— rock matrix porosity accessible to
-	the parent radionuclide p (dimensionless)
D_i	— pore water diffusion coefficient
	for radionuclide <i>i</i> (L^2/T)
\bar{c}_i	— concentration of radionuclide i in the pore-water
L	in the rock matrix (M/L^3)
Z	— direction perpendicular to the flow direction
_	into the rock matrix (L)
R	— retardation coefficient (dimensionless)
11	retartation coefficient (unitensioness)

The boundary and initial conditions are

$$-\frac{\alpha L^2}{t_w} \frac{\partial c_i}{\partial x}\Big|_{x=0} A + \frac{L}{t_w} c_i(x=0)A = r_i$$
[3]

$$\bar{c}_i(z=0) = c_i$$
 at all times [4]

$$c_i(t=0) = \bar{c}_i(t=0) = 0$$
[5]

$$\left. \frac{\partial \bar{c}_i}{\partial z} \right|_{z=12.5 \text{ m}} = 0 \tag{6}$$

$$c_i(x \to \infty) = 0 \tag{7}$$

where

A— fracture cross section perpendicular
to the flow direction
$$(L^2)$$
 r_i — near-field release rate (M/T)

The far-field release rate (release rate into the biosphere) is computed as

$$r_i^{out} = -\frac{\alpha L^2}{t_w} \left. \frac{\partial c_i}{\partial x} \right|_{x=L} A + \frac{L}{t_w} c_i (x=L)A$$
[8]

The fracture semi-aperture, b, is computed as

$$b = \frac{t_w}{F}$$
[9]

where F is the transport resistance factor in T/L units. By expressing the mass conservation equations with dimensionless units, it is possible to show that the far-field release rate in Eq. [8] is independent of the pathway length, L, and the cross section, A. Accordingly, SKB does not provide values for those parameters.

For stochastic simulations, SKB provides values in Table 4-3 of the Radionuclide Transport Report for the canister failure time, the rock transport resistance (F), the advective travel time (t_w), and the advective flow through the deposition hole (q). SKB used those discrete values repeatedly in the multiple-realization computations for the stochastic simulations. In our model, we opted for a different approach. We established cumulative distribution functions for $\log(F)$, $\log(t_w)$, and q, and performed continuous interpolation to sample values for input parameters for the stochastic simulations. The failure time in Table 4-3 of the Radionuclide Transport Report is nearly uniformly distributed. Accordingly, we sampled the failure time from a uniform distribution ranging from 114,486 yr to 978,463 yr (i.e., minimum and maximum times in Table 4-3). We sampled the failure time, $\log(F)$, and q independently from each other because Table 4-3 of the Radionuclide Transport Report suggested weak correlations between these parameters. A correlation coefficient between $\log(F)$ and $\log(t_w)$ equal to 0.88 was computed from Table 4-3 of the Radionuclide Transport Report and was preserved in the sampling for the stochastic simulations.

3.2. Results and discussion

We derived reasonable visual agreement with SKB results in terms of the magnitude and trend of near-field and far-field doses for our deterministic and stochastic simulations (Figure 2). For the central corrosion case (i.e., the SKB case assuming no solubility limits except for very low solubility for thorium, as illustrated by Figures 4-2 to 4-5 in the Radionuclide Transport Report), our radionuclide release rates matched the near-field and far-field release rates (see Figure 2). However, we had to assume extremely low solubility for both uranium and thorium. Such an assumption, which corresponds to near-zero aqueous concentrations of uranium and thorium, causes uranium and thorium isotopes to be retained almost completely within the canister, so the resulting large inventory of uranium and thorium that is available for decay in the canister maximizes the near-field releases of Ra-226 and Pb-210. Values of the partition coefficient (K_d) for radium in the geosphere are relatively low; and the advective water travel time through the geosphere is brief (only a few years), so the release rates for Ra-226 after transport through the geosphere are only slightly lower than the near-field release rates for Ra-226.

The initial release of Se-79 after canister failure, as illustrated in Figure 2(a), is greater than SKB's calculated release (e.g., Figure 4-2 of the Radionuclide Transport Report). We could only match the initial SKB Se-79 release by decreasing the initial Se-79 inventory with respect to values that SKB suggested in the Data Report (Table 3-3). The reason for this discrepancy is unclear, but it raises a question about the initial Se-79 inventory adopted in the SKB computations.

The results of the stochastic simulations, shown in Figures 2(c) and 2(d), are in reasonable agreement with the SKB results. In the stochastic simulations (200 realizations), we assumed that a single canister would fail by corrosion, at a time sampled from a uniform distribution ranging from 115,000 to 1,000,000 years. We applied a dose factor of 0.12 to the dose computations to account for the SKB statement that after one million years, an average of 0.12 canisters would have failed by corrosion.

The verification of stochastic computations indicates that the waste form degradation rate plays a major role in controlling releases to the near field and far field, and it is positively correlated to dose estimates. Large values of the geosphere transport resistant factor, F, and the water travel time, t_w , cause doses to be reduced; thus, F and t_w are negatively correlated to dose estimates. Stochastic runs with late canister failure times are associated with low dose estimates. Therefore, the canister failure time is also negatively correlated to dose estimates. From a correlation analysis to the far-field dose at one million years, we developed the following ranking of input parameters:

- (1) Spent fuel degradation rate (correlation = 0.58)
- (2) Log(F) (correlation = -0.47)
- (3) $\text{Log}(t_w)$ (correlation = -0.38)
- (4) Canister failure time (correlation = -0.217)

This ranking and the correlation signs are consistent with the sensitivity results in Figure 4-7 of SKB's Radionuclide Transport Report.

SKB has computed variants of the unlimited solubility case. For example, in Figures 4-12 to 4-15 of the Radionuclide Transport Report, SKB provided results assuming unlimited solubility for all radionuclides except uranium. (We had to assume almost 0 solubility for uranium to match SKB results). Results of the verification computations are provided in Figure 3. In Figure 4-16 to 4-18 of the Radionuclide Transport Report, SKB provided dose results assuming finite and non-zero solubility limits. For deterministic computations, we used solubility limits from Table 3-4 of the Radionuclide Transport Report, except for uranium (for which we assumed an arbitrarily small solubility). For stochastic computations, we digitized the distribution functions SKB provided in Figures F-21, F-22, F-23, F-25,

Figure 2: Results of the verification modelling of the scenario for canister failure by corrosion (top), contrasted with SKB model results (bottom) for the same case: (a) Near-field releases, (b) Far-field releases, (c) Near-field releases, stochastic case, (d) Far-field releases, stochastic case, and (e) Confidence interval on the far-field dose estimate. All of the verification results assumed unlimited solubility for all modelled radionuclides except that very low solubility (almost zero) was assumed for U and Th. Figures at the bottom (with their original figure numbers retained in the reproduced captions) are from SKB's Radionuclide Transport Report. The header of each figure at the top cites the comparable SKB figure number from the Radionuclide Transport Report that is reproduced at the bottom.











Figure 3: Results of the verification modelling of the scenario for canister failure by corrosion (top), considering unlimited solubility for all modelled radionuclides except that very low solubility (almost zero) was assumed for uranium: (a) Near-field releases, (b) Far-field releases, (c) Near-field releases, stochastic case, and (d) Far-field releases, stochastic case. Figures at the bottom are the corresponding SKB model results for the same cases that were presented in SKB's Radionuclide Transport Report, with the original SKB figure numbers retained in the reproduced captions. (The header of each figure at the top cites the corresponding SKB figure number from the Radionuclide Transport Report that is reproduced at the bottom.)









F-27, F-28, F-29, F-33, F-34, and F-35 of Appendix F of the Radionuclide Transport Report, and we input those distributions as look-up tables into the GoldSim model to be sampled by interpolation. We noted that median values of the distribution functions in Appendix F are not in agreement with presumably median values in Table 3-4 of the Radionuclide Transport Report. As in previous cases and as previously stated, we assumed an arbitrarily small solubility for uranium to match the SKB results. This zero-uranium-solubility assumption is not described by SKB in its documentation. Results of the verification computations are included in Figure 4. The results are comparable in magnitude and trend to SKB results.

We noted a few differences with the SKB results. For example, in Figure 4(a), the Tc-99 near-field release curve is initially flat due to solubility constraints. Such flat release is not observed in the SKB computations in Figure 4-16 of the Radionuclide Transport Report. In the stochastic simulation results in Figure 4(c), the high Pb-210 releases are due to the retention of Ra-226 in the near field due to precipitation, increasing the production of Pb-210 by ingrowth. To force Ra precipitation, we decreased the solubility distribution in Figure F-28 in Appendix F of the Radionuclide Transport Report by a factor of 1,000. This factor of 1,000 decrease is justified to account for Ba-Ra co-precipitation. However, in the SKB documentation it is not clear whether the 1,000 decrease factor is already embedded in the solubility distribution in Figure F-28. The description in Appendix F appears to imply that a factor of 1,000 is already part of the SKB distribution; however, we had to apply the factor in addition to the distribution to derive results comparable to SKB.

4. Scenario for canister failure by shear load

SKB considers that seismic events could cause fractures intersecting deposition holes to displace and possibly cause failure of the canister by shear. SKB proposed to implement a "respect distance" concept to avoid fractures of a critical size that could significantly displace after a seismic event and cause canister failure. Thus, in this scenario, the number of canisters that could fail is determined by undetected fractures exceeding a critical size intercepting deposition holes, or by errors in locating and avoiding critical fractures during repository construction. SKB modelled this scenario by (i) assuming failure of the canister at an arbitrary time between 1,000 and one million years, (ii) assuming that the buffer material is a diffusion barrier against radionuclide transport, and (iii) not taking any credit for the presence of the canister or radionuclide transport in the geosphere. In this section, we discuss the simplified model we used to approximate the SKB computations for the scenario for canister failure by shear load is discussed, and we compare the model results to the SKB results.

4.1. Model setup and assumptions

The near-field model elements of the SKB scenario for Canister Failure by Shear Load in the Radionuclide Transport Report are summarized in Figure 5. The descriptions for the waste form component, the in-canister water volume, the initial inventories, and the IRF and CRF are the same as the descriptions for the scenario









Figure 5: Model elements of the near field in the scenario for Canister Failure by Shear Load



for canister failure by corrosion in Section 3 of this technical note. The scenario for failure by shear load scenario includes buffer material as a diffusion barrier for radionuclide transport. The diffusion barrier was not used in the corrosion scenario, where it was assumed that the buffer already had been eroded away. In the cylindrical buffer, radionuclides would diffuse along the radial and vertical directions and then would be carried away by water flowing around the buffer. We implemented two simplifications in the model: we ignored vertical diffusion along the buffer, and we approximated the cylindrical buffer as a slab with a constant cross section thickness of 25 cm. We considered equilibrium linear sorption in the diffusion transport computations. Accordingly, the mass balance equation for radionuclide *i* in the buffer is

$$R_i \frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial r^2} - \lambda_i c_i R_i + \lambda_p c_i R_p \frac{\theta_p M_i}{\theta_i M_p}$$
[10]

This equation is similar to Eq. [2], except that concentrations, diffusion coefficients, and retardation coefficients refer to quantities in the buffer. The variable r represents the radial direction. The boundary condition at the buffer terminus is

$$-\theta_i D_i \left. \frac{\partial c_i}{\partial r} \right|_{r=0.25 \text{ m}} A_b = c_i (r = 0.25 \text{ cm})q$$
^[11]

where $q = 1 \text{ m}^3/\text{yr}$ is the assumed flow through the deposition hole and A_b is the cross section of the buffer slab perpendicular to the diffusive transport direction.

The concentration c_i at r = 0.25 m is established by solving the differential mass balance equation. Equation [11] is also used to compute the near-field radionuclide releases rate in mass/time (M/T) units. The SKB model ignores transport in the geosphere; thus, the far-field radionuclide release rates are assumed to be equal to the near-field release rates. At the position r = 0, the concentration gradient is controlled by the rate of degradation of the waste form and by solubility limits.

Consistent with the SKB model description, we implemented solubility constraints in the buffer material. The implementation was similar to our implementation of solubility constraints in the in-canister water for the scenario for Canister Failure by Corrosion (Section 3). We adopted a split operator algorithm in which diffusion transport in the buffer is computed first at a computer timestep, and then solubility limits are enforced in the same timestep. We derived almost identical radionuclide release rates from the buffer for cases enforcing solubility limits in both the in-canister water and the buffer compared to cases enforcing solubility limits in the in-canister water only. Therefore, it appears that when solubility limits are considered, it is sufficient to enforce those limits in the in-canister water, and ignore those limits in the buffer material. In computations reported herein for cases considering solubility limits, the solubility limits were enforced in both the in-canister water and the buffer material for consistency with the SKB description.

Our numerical results indicate buffer release rates were nearly independent of the assumed deposition hole flow, q. The assumed flow of $q = 1 \text{ m}^3/\text{yr}$ is high enough that any assumed higher flows would not significantly change the near-field release rates. On the other hand, near-field release rates are dependent on the cross section A_b . We used a cross section $A_b = 2.1 \text{ m}^2$, which was computed using data in Table G-6 of Appendix G of the Radionuclide Transport Report. We used the inner radius of 0.675 m and a block height of 0.5 m to calculate the cross section as $2 \pi (0.675 \text{ m}) (0.5 \text{ m}) = 2.1 \text{ m}^2$. The buffer block height of 0.5 m seems somewhat arbitrary, given that SKB specifies that the canister height is 4.835 m. Given the apparent dependence of near-field release rates on the buffer height parameter, it would be helpful for SKB to provide a technical basis to justify the selection of the buffer block height as 0.5 m.

4.2. Results and discussion

Results of the deterministic and stochastic (200 realizations) simulations are presented in Figure 6. We derived trends and magnitudes in release rates that were similar to SKB results. Some slight differences are noted. For example, the flat release rate in the Se-79 release rate at around 100,000 years in Figure 6(a) is due to solubility constraints. This solubility limited Se-79 release rate is not evident in the SKB computations (Figure 5-1 of the Radionuclide Transport Report). We derived reasonable agreement in the I-129, Nb-94, Np-237 and Tc-99 releases from Figure 5-1 of the Radionuclide Transport Report. We could match the Pu-242 releases by assuming a lower value of the K_d for Pu than the value recommended in Table 3-3 of the Radionuclide Transport Report. The magnitude of the Ra-226 and Th-230 releases in our computations is larger than the SKB results. We could not reproduce the up-and-down trend in the Th-230 and Ra-226 releases. The up-anddown trend is intriguing, as it may indicate depletion of Th-230 inventory; however, Th-230 is supported by U-234 and by U-238, which are not depleted. The Swedish Radiation Safety Authority (SSM) may wish to ask SKB to provide a clarification on the factors controlling the up-and-down trend in the release rate of Th-230. Supplemental information in the form of release rates from the in-canister water into the buffer material, and radionuclide concentration and precipitated mass in the in-canister water also would help in interpreting SKB's near-field release rate trends.

Results of stochastic simulations (200 realizations) are provided in Figure 6(b). In our computations, we included the IRF, but SKB did not, which accounts for the taller spike in our computations. The results are in reasonable agreement with the SKB results (Figure 5-2 of the Radionuclide Transport Report). SKB's up-and-down trend in the release rate of Th-230 could not be reproduced in our simplified computations. We could match the Pu-242 release rate only by lowering the K_d values for Pu recommended by SKB in Table 5-16 of the Data Report. Supplemental information by SKB on the K_d values used in their computations would help in resolving the discrepancy.

Figure 6: Results of the verification modelling of the scenario for Canister Failure by Shear Load (top) contrasted with the corresponding SKB model results for the same cases, as presented in SKB's Radionuclide Transport Report: (a) deterministic run, (b) stochastic run with a single canister failure at a fixed time, (c), stochastic run with random canister failure time, (d) to (f) stochastic runs with random canister failure time for a case assuming the buffer is not present. (The header of each figure at the top cites the corresponding SKB figure number from the Radionuclide Transport Report that is reproduced at the bottom.) In the modelling, SKB assumed near-field and far-field releases are equal.












Results of stochastic simulations (200 realizations) sampling the canister failure time from a uniform distribution ranging from 1,000 to 1,000,000 years is presented in Figure 6(c). We obtained results that were comparable to those of SKB. Neither our computations nor those of SKB included the IRF in the release rates. Our release rates for Ra-226 were higher, but the release rates for I-129, Se-79, and Nb-94 were of similar magnitude. We derived fluctuating release rates for C-14 due to the consideration of a relatively small number of realizations. However, our results are in agreement with the SKB results indicating that early releases (in the first few thousands of years) are dominated by C-14. In the stochastic simulations, we assumed one canister to fail at a random time in every realization. However, we

applied a factor of 0.079 to the dose estimates to account for the SKB assertion that at one million years, an average of 0.079 canisters is expected to fail by shear load.

SKB considered a special case where the buffer material was absent. This case was equivalent to the scenario for Canister Failure by Corrosion. The only difference was that the deposition-hole flow rate was constant in the shear load computations (equal to $1 \text{ m}^3/\text{yr}$), as opposed to sampled values in the Canister Corrosion scenario. For the sake of simplicity, we used the same model as the Canister Failure by Corrosion scenario, and we sampled the canister failure time from a uniform distribution from 1,000 to 1,000,000 years. Results are presented in Figure 6(d)-(f). The late releases of Np-237, I-129, Se-79 are similar to the SKB results, as presented in Figure 5-7 of the Radionuclide Transport Report. Our Ra-226 releases are higher than the SKB results. Our Pb-210 releases are also higher; however, this was expected because the stochastic computations used smaller deposition hole flow rates than the flow rate of $1 \text{ m}^3/\text{yr}$ used by SKB. (Use of low flow rates causes the Pb-210 to trail the Ra-226 release rates; high flow rates cause Pb-210 release rates to decrease with respect to Ra-226 release rates.) In Figures 6(e) and (f), the simulation period was narrowed to the first 100,000 years and to the first 10,000 years, respectively, to produce smoother release rate curves. In generating both sets of results 200 realizations were considered, and the failure time was selected from uniform distribution functions ranging from 1,000 to 100,000 years, and from 1,000 to 10,000 years, respectively. Our results were in agreement with the SKB results in predicting that the early doses would be dominated by Nb-94 and C-14. In contrast, the C-14 release rates we computed are greater than the corresponding SKB release rates. We assumed that one canister failed at a random time in every realization, then we applied a factor of 0.079 to dose estimates to account for the SKB estimation that within one million years, an average of 0.079 canisters is expected to fail by shear load.

Using the data for the run presented in Figure 6(c), we computed correlation coefficients to the dose at one million years, and we found only two parameters that were significantly correlated with the dose estimates. The spent fuel degradation rate had a positive correlation of 0.83, and the canister failure time had a negative correlation of -0.41.

These results are only partially consistent with SKB results of a sensitivity analysis presented in Figure 5-4 of the Radionuclide Transport Report because SKB also found that the solubilities of Ra and Th are correlated to the dose at one million years. However, on page 117 of the Radionuclide Transport Report, SKB argues that disregarding Ra solubility constraints only increases the dose by a small factor. On page 118 of the same report, SKB argues that increasing the Ra solubility by a factor of 1,000 increases the Ra release rate only by a factor of 1.5. Therefore, it is unclear why SKB detected the Ra solubility as an important parameter in its sensitivity analysis. With respect to the sign of the sensitivity index for the solubility of Th, SKB reports the sign to be positive, but that statement is counter-intuitive. Low solubility of Th implies retention of Th-230 in the near-field, which would cause an increase in the mass and release rate of Ra-226. Accordingly, the sign of the sensitivity index would be expected to be negative. A clarification is needed by SKB on why the Ra solubility was identified as an important parameter if increasing the solubility by a factor of 1,000 only marginally increases the dose. Also, clarification is needed on why the sign of the sensitivity index for the solubility of Th is positive, when based on the results for the other scenario. Canister Failure by Corrosion, the sign of the index was expected to be negative.

A spot check reveals inconsistencies in values in different reports [e.g., the data used in determining inclusion/exclusion of radionuclides and data for actual transport calculations]. For example, SKB reports two different values for the half-life of Th-229 (7,880 yr in Table 3-5 of the Data Report, and 7,340 yr in Table D-2 of the Radionuclide Transport Report). Likewise, Table D-2 of the Radionuclide Transport Report uses a half life of 4,320 yr for Am-241 whereas Table 3-5 of the Data Report uses a half life of 432.7 yr. The differences may point to some potential errors if both values have been used in calculations.

5. Conclusions

We calculated release rates that were comparable, in magnitude and trend, to SKB computations for the scenario of canister failure by corrosion. However, to derive similar results we had to assume almost zero uranium solubility for all of the corrosion cases. Assuming zero solubility for uranium and thorium resulted in maximum releases of Ra-226 from the near field. It is not clear from the SKB documentation whether SKB used a similar assumption or adopted solubility values as in Figure F-35 of the Appendix F and Table 3-4 of the Radionuclide Transport Report. Also, the distribution of Ra solubility values for the stochastic computations is unclear. To derive results that were comparable to those in Figure 4-18 of SKB's Radionuclide Transport Report, we decreased the Ra solubility by a factor of 1,000 compared to the distribution in Figure F-28 of Appendix F of the Radionuclide Transport Report. We suggest that SKB provide appropriate clarification about the deterministic and stochastic values of the solubility limits used in the SKB computations, including solubilities for U, Ra, and Tc. If uranium was assumed to have an arbitrarily low solubility, SKB needs to provide a technical basis to justify such an assumption in the computations. Additional information about SKB's choice of values for the initial Se-79 inventory would be useful in interpreting slight differences we observed in attempting to reproduce SKB's near-field releases from Figures 4-2 and 4-12 of the Radionuclide Transport Report.

The results we derived for the canister failure by shear load scenario were comparable overall to those of SKB. We suggest that SKB be asked to clarify the basis for the values used for Se solubility and for the Pu K_d used in the SKB computations. Also, it is unclear why SKB results for Th-230 and Ra-226 show up-and-down trends (decreasing trends imply Th-230 depletion). We also question why SKB identified Ra solubility as an important factor in its sensitivity analysis, and why the sign of the sensitivity index of the Th solubility is positive. SKB also may need to explain the rationale for specifying a height of 0.5 m for buffer material in the SKB computations. These suggested requests for complementary information are listed in Appendix 2.

Our verification computations for the scenario for Canister Failure by Corrosion and the scenario for Canister Failure by Shear Load confirmed SKB's observation that the rate of waste form degradation plays a major role in the safety assessment: SKB considers that waste form degradation under reducing conditions is a slow process, ranging from a million to a hundred million years. In the SKB performance assessment computations, the concentrations of radionuclides in the water inside the canister that can be released after canister breach, in particular U-238, U-234, Th-230, Ra-226, and Pb-210, are constrained by the rate of waste form degradation. However, an additional contribution to the near-field release of Pb-210 could come from the *non-degraded* waste form due to Rn-222 arising from decay of Ra-226 in the non-degraded waste form. Such Rn-222 could escape as part of the gas phase

after a canister breach and decay to Pb-210. This potential additional release of Pb-210 is not accounted for in the SKB computations. The Pb-210 could then be transported from the near field to the biosphere along with the Pb-210 currently tracked by the SKB computations. Within the scope of this initial review, it was not clear whether such a contribution to the Pb-210 releases would be dominant or negligible. As detailed in Appendix 2, we recommend that SKB conduct additional investigative analyses to assess the significance of this omitted contribution from Pb-210 and its potential impact on the safety case.

6. References

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SKB. "Radionuclide transport report for the safety assessment SR-Site." TR-10-50. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. 2010a.

SKB. "Data report for the safety assessment SR-Site." SKB TR-10-52. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. 2010b.

Appendix 1: Coverage of SKB reports

Table A-1 summarizes the reports covered in this review activity, with a brief description on the information consulted.

Table A-1:	List of SKB reports	s consulted for the	verification of computations
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Reviewed report	Reviewed sections	Comments (Information Consulted)
TR-10-11: Long-term safety for the final repository for spent nuclear fuel at Forsmark: main report of the SR-Site project		Volume III, Chapter 13 Information consulted to gain a general understanding of the SKB safety assessment and main components affecting dose estimates
TR–10–50: Radionuclide transport report for the safety assessment SR-Site. Technical Report		 Description of computations for Canister Failure by Corrosion (Chapter 4) and Canister Failure by Shear Load (Chapter 5) Input data for deterministic simulations (solubility, K_d) Dose estimates to compare to independent computations Appendix F for solubility data for stochastic simulations Appendix G for description of system geometry and dimensions for shear load failure computations
TR–10–52: Data report for the safety assessment SR-Site		 Inventories and half-lives Instant and corrosion release fractions Waste form degradation rate and corrosion degradation rate Diffusion coefficients, porosities, and partition coefficients for buffer material Diffusion coefficients, porosities, and partition coefficients for rock matrix Landscape dose factors
R–09–56: MARFA version 3.2.2 user's manual: migration analysis of radionuclides in the far field		 Definition of transport resistance factor Equations for matrix diffusion
R–04–64: COMP23 version 1.2.2 user's manual		 Mass balance equations for near field, including waste form dissolution, solubility constraints, and decay and ingrowth
TR-10-42: Mass transfer between waste canister and water seeping in rock fractures—Revisiting the Q-equivalent model, I. Neretnieks, L. Liu, L Moreno, Royal Institute of Technology, KTH, March 2010		Transport resistance factor

Appendix 2: Suggested needs for complementary information from SKB

Rn-222 Gas Releases Not Constrained by Waste Form Degradation

The rate of waste form degradation plays a major role in the Swedish Nuclear Fuel and Waste Management Company (SKB) computations for the Canister Failure by Corrosion and Canister Failure by Shear Load scenarios. SKB considers waste form degradation under reducing conditions to be a slow process, ranging from one-million to one-hundred million years. In the SKB performance assessment computations, radionuclides in the water inside the canister that could be eventually released into the environment after a canister breach, in particular U-238, U-234, Th-230, Ra-226, and Pb-210, are constrained by the rate of waste form degradation. Potential additional contribution to the near-field Pb-210 release from the nondegraded waste form should be examined further. Because Rn-222 arising from decay of Ra-226 will be present in the non-degraded waste form, it could escape in gas phase into the near field following a canister breach, and decay to Pb-210 (the half-live of Rn-222 is 3.8 days). Once in the near field, Pb-210 could be transported to the biosphere, in addition to the Pb-210 currently tracked by the SKB computations. At this time it is not clear whether such contribution to the Pb-210 releases is dominant or negligible. SKB should analyze this potential additional Pb-210 release, or provide a technical basis on why its inclusion in the performance assessment is unnecessary.

Clarification Questions on Radionuclide Transport Computations and Sensitivity Analyses

Independent modelling has verified a limited set of SKB computations that SKB described in Chapters 4 and 5 of the Radionuclide Transport Report (TR-10-50; SKB, 2010). The SKB results were successfully reproduced to a degree of accuracy, but specific divergences were noted in the results in a number of instances. Our general observation is that the SKB radionuclide transport computations for performance assessment are sound and are consistent with radionuclide transport computation approaches in performance assessments carried out by other international organizations in radioactive waste management and geological disposal. The SKB descriptions of radionuclide transport computations are detailed enough to allow an experienced reviewer to reproduce computations. Although the identified divergences do not appear to be significant enough to alter SKB conclusions in the safety case, we suggest that The Swedish Radiation Safety Authority (SSM) follow up with SKB to obtain complementary information about some of the specific divergence and transparency issues. This would provide a helpful perspective for SSM's review of the safety case by determining whether the SKB divergences result from errors or simply from a lack of information in the descriptions that SKB has provided so far. The additional information is needed for a better understanding of the SKB safety assessment and to enhance confidence in SKB computations. The clarification questions are numbered from 1 to 4 as follows.

 Input data (solubility for U, Ra, Tc, and Se; initial Se-79 inventory; buffer material Pu K_d) used in computations in the Radionuclide Transport Report (TR-10-50; SKB, 2010) are unclear. The technical basis for the selection of U solubility values for the Canister Failure by Corrosion computations (Chapter 4 of the Radionuclide Transport Report) is unclear. In independent computations, arbitrarily small solubility for U was required to be adopted to approximate SKB results in Figures 4-2, 4-4, 4-12, 4-14, 4-16, and 4-18. The SKB description with regards to U solubility is confusing as SKB labelled its cases as "no solubility limits" and "including solubility limits in the near field," yet it appears that SKB assumed extremely low solubility for U throughout, with values well below those in Figure F-35 of Appendix F of the Radionuclide Transport Report. SKB should clarify values of the U solubility used in its deterministic and stochastic computations for the aforementioned figures, as well as provide a technical basis in case U solubility values in the computations differ from those in the Appendix F (Figure F-35) of the Radionuclide Transport Report.

In the case of Figure 4-18, comparable results to SKB's were derived in independent computations by decreasing solubility limits for Ra (Figure F-28 in Appendix F of the Radionuclide Transport Report) by a factor of 1,000. SKB should clarify whether or not the factor of 1,000 to account for Ba-Ra co-precipitation is embedded in the distribution in Figure F-28 of the Appendix F.

In the case of Figure 4-16, independent computations suggest significant precipitation of Tc shortly after canister failure, for at least 10,000 years, yet such precipitation is not evident in the SKB computations. In the independent computations, the recommended value of Tc solubility in Table 3-4, page 52 was used. SKB should clarify the Tc solubility used in the computations for Figure 4-16.

In the case of Figure 5-1, the independent computations suggest precipitation of Se shortly after canister failure lasting for few tens of thousands of years, but such precipitation is not evident in the SKB computations. The recommended value of Se solubility in Table 3-4, page 52, was used in the independent computations. SKB should clarify the Se solubility used in the computations for Figure 5-1.

In the verification computations for Figures 4-2 and 4-12 of the Radionuclide Transport Report, the initial Se-79 releases resulted slightly above the SKB results. One possible explanation for the divergence is the use of different initial inventories in the independent verification computations and the SKB computations. The independent computations used the initial inventory recommended in Table 3-3 of the Data Report (TR–10–52). SKB should clarify the initial Se-79 inventory used in its computations.

In verifying results reported in Figures 5-1 and 5-2, Pu-242 release rates could be approximated by assuming lower values for the buffer material Pu K_d than recommended in Table 3-3 of the Radionuclide Transport Report (deterministic computations) and Table 5-16 of the Data Report (stochastic computations). SKB should clarify values of Pu K_d used in its computations for Figures 5-1 and 5-2 of the Radionuclide Transport (SKB, 2010).

2. Release rate trends of Th-230 and Ra-226 in Figures 5-1 and 5-2 of the Radionuclide Transport Report are not intuitive.

In the verification computations, the decreasing trends for release rates of Th-230 and Ra-226 in Figures 5-1 and 5-2 could not be reproduced. In the

independent verification computations, the release rates increase and then plateau. SKB should explain the decreasing trend in the Th-230 releases, which appears to imply depletion of Th-230 in the system. SKB should include intermediate results such as release rates from the in-canister water into the buffer material, and radionuclide concentration and precipitated mass in the in-canister water, to supplement information to facilitate understanding of the trends in the SKB computations.

3. Sensitivity analysis results in Figure 5-4 of the Radionuclide Transport Report are not intuitive.

It is not clear why the SKB sensitivity analysis (Figure 5-4 of the Radionuclide Transport Report) identified the Ra solubility as an important parameter, as it appears in contradiction with SKB explanations suggesting that Ra solubility is not important. For example, on page 118 of the Radionuclide Transport Report, SKB argues that increasing the Ra solubility by a factor of 1,000 increases the Ra release rate only by a factor of 1.5. SKB should clarify whether Ra solubility is or is not relevant to stochastic dose estimates of the shear load scenario.

The sign of the sensitivity index (+) in Figure 5-4 associated with Th solubility is confusing. From the verification computations, it was noted that increasing retention of Th in the near field (for example by using low solubility values for Th) would increase the Ra-226 release. Therefore, low Th solubility values would be associated with high Ra-226 releases and high-doses. SKB should explain the sign of the sensitivity index for Th solubility derived from its sensitivity analysis.

4. Dose estimates for the shear load scenario appear to depend on the model discretization.

In the verification computations, near-field release rates were dependent on the assumed height of the buffer material block (0.5 m according to Table G-6 of the Appendix G of the Radionuclide Transport Report). The SKB technical basis for selecting a height of 0.5 m is unclear. SKB should state whether its results depend on this 0.5-m length parameter, and, if so, SKB should provide a technical basis for selecting this length of 0.5 m for the computations reported for the scenario for Canister Failure by Shear Load in Chapter 5 of the Radionuclide Transport Report.

Reference

SKB. "Radionuclide transport report for the safety assessment SR-Site." TR-10-50. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. 2010.

Appendix 3: Suggested review topics for SSM

Rn-222 Gas Releases Not-Constrained by Waste Form Degradation

In Appendix 2, a mechanism for release of Rn-222 leading to a contribution of Pb-210 in addition to the concentration tracked in the Swedish Nuclear Fuel and Waste Management Company (SKB) computations is presented. We suggest that The Swedish Radiation Safety Authority (SSM) evaluate potential additional releases of Pb-210 arising from transport of Rn-222 in gas phase and eventual decay to Pb-210 in the near field.

Alternative Waste Form Dissolution Model

The rate of waste form degradation plays a major role in the SKB computations for the Canister Failure by Corrosion and Canister Failure by Shear Load scenarios. An alternative model for radionuclide release from the waste form can be developed by assuming release controlled by the solubility of the waste form matrix. The waste form could be assumed in thermodynamic equilibrium with the in-canister solution. The waste form matrix would dissolve in this model only when concentration in solution is below a solubility limit. In this alternative model, the rate of transport of the dissolved waste form matrix may be the rate controlling step, as well as the solubility of the uranium matrix. Note that infinitely fast dissolution and precipitation kinetics is implicitly assumed to enforce thermodynamic equilibrium in the alternative model. On the other hand, the chemical kinetics of waste form dissolution is expected to be very slow in the physical system, especially in reducing waters. Thus, solubility control (as opposed to kinetic control) of waste matrix dissolution may be a conservative approach to model waste form dissolution and release of radionuclides to the environment. We suggest that SSM analyze further this alternative model for waste form dissolution, given the significance of waste form dissolution in the SKB performance assessment computations.

Number of Canisters Failed and Time of Failure for Corrosion and Shear Load Failure Scenarios

The number of canisters breached and the breach time are two important factors in the SKB dose estimates. Given the risk significance of these factors, we recommend that SSM support its review by conducting a set of verification computations of the number of canisters breached in the corrosion failure scenario. It is necessary to verify the dependence between the fraction of canisters failed and the chemical composition (and spatial and temporal variability) of groundwaters. Computations involving discrete fracture networks (DFN), and the number of water-carrying fractures intercepting deposition holes and causing significant buffer erosion and then corrosion of the canister, should be evaluated in detail in regards to how they affect the number of canisters breached. The probability of early canister failure, for example due to localized corrosion, creep, or stress corrosion cracking, should be accounted for in the independent analyses.

It is also recommended that SSM verify SKB computations to estimate the number of canisters breached in the shear load scenario. The verification computations should consider frequency of seismic events, DFN, critical size fractures, and respect distances to deposition holes, as well as uncertainties in the shear load failure analysis and initiating seismic events.

Impact of Flow Parameters on Geosphere Radionuclide Transport Calculations

SKB provides flow model output information (i.e., advective travel times and flow-related transport resistance parameters for individual transport pathways) as input to the radionuclide transport model. At a median value of 21.6 years (some values as low as 6 years) (see Table 4-3, TR-10–50; SKB, 2010), the advective travel time appears to be too pessimistic, and at a median value of 102,920 years (see Table 4-3, TR-10–50; SKB, 2010); the transport resistance factor appears to be too optimistic. The net effect of the use of pessimistic and optimistic values for the water travel time in the overall SKB performance assessment computations is not clear. Therefore, we recommend SSM to carry out verification calculations of flow parameters. SKB calculations on water travel time and transport resistance for radionuclide transport calculations should be verified, and independent detailed computations should be carried out to evaluate data support and propagation of uncertainty in the SKB analyses.

Impact of the Variation of Radionuclide Inventory Emplacement in the KBS–3 Repository

SKB calculations show sensitivity to the average initial radionuclide inventory (see Appendix E of TR–10–50; SKB, 2010). Inventories could vary from location to location in the repository and from canister to canister, and SKB has pointed out the possibility of inventory variation around the mean by a significant amount, which could affect dose estimates. For example, SKB notes that the Ag-108m, which contributes significantly to dose associated with the hypothetical case of shear failure with early failure of pressurized water reactor canisters, can have a factor of four higher inventory than the assumed average. In the independent model verification effort to date, we have conducted analyses using only a short list of radionuclides, and the calculations did not address uncertainty in the inventory. SSM should consider conducting verification analyses using inventory variations to obtain a more detailed understanding of the impacts on dose.

Modelling other Scenarios (Pinhole Scenarios and Colloidal Transport)

In the independent model verification study, attention focused on two scenarios: failure of the copper canister by corrosion and by earthquake-induced shear movements in fractures intersecting the canister positions. These were the new scenarios considered after the SR-Site, compared to the pinhole release scenario in the SR-Can. It is recommended to verify computations for the pinhole and growing pinhole scenarios. In addition, it is recommended to review the treatment of colloidal transport, as such kind of radionuclide transport could give rise to early breakthrough.

Degraded Barrier Performance Analysis

SKB conducted a variety of sensitivity analyses and barrier-off analyses to illustrate barrier capability (Sections 6.4 and 6.5, TR-10-50; SKB, 2010). The barrier capability analysis was done by neutralizing barriers or reducing their barrier capabilities. We recommend carrying out systematic barrier degradation analysis (not full barrier neutralization) in which the performance uncertainty is evaluated at various specified levels of degradation of barrier components that could be attainable. From the perspective of SSM, the objective of this analysis would be to systematically evaluate the degree of confidence on average dose estimates and their

separation from compliance risk limits and to estimate the combination of barrier component degradations that would lead to the average dose estimates to exceed the risk limit. The smaller the probability of getting such component degradations, the greater is the confidence in the safety conclusions. This combined barrier degradation analysis could be interpreted as an enhanced uncertainty analysis, beyond input parameter uncertainty and barrier neutralization analysis.

Reference

SKB. "Radionuclide transport report for the safety assessment SR-Site." TR-10-50. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. 2010.

2012:58

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.

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