Modeling in Support of SSM's Licensing Review of a Geological Repository for Spent Nuclear Fuel – 14164

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ABSTRACT

In 2011 the Swedish Nuclear Fuel & Waste Management Co. (SKB) submitted a license application for construction of a spent nuclear fuel repository. The license application is supported by a post-closure safety assessment, SR-Site. Together with other parts of the application, SR-Site is currently being reviewed by the Swedish Radiation Safety Authority (SSM). One element of SSM's review is independent modeling. In this paper we describe how this modeling is performed and the findings that have been obtained from the initial phase of SSM's licensing review. The findings from the modeling have been used to identify critical issues for further in-depth review and to develop requests for clarifications and complementary information from SKB concerning their reporting of post-closure safety. In this paper we focus on independent modeling of the *consequence analysis* in SR-Site.

INTRODUCTION

In 2011 the Swedish Nuclear Fuel & Waste Management Co. (SKB) submitted a license application for construction of a geological repository for spent nuclear fuel at Forsmark. SKB's disposal method, the KBS-3 method, involves disposing of the spent nuclear fuel in cast iron canisters with 0.05 m lining of copper. The canisters will be placed in vertical deposition holes at approximately 500 m depth in crystalline bedrock. Each canister is surrounded by a buffer of swelling bentonite clay. The repository is designed to accommodate 6 000 canisters, corresponding to 12 000 tons of spent nuclear fuel.

The license application is supported by a post-closure safety assessment, SR-Site [1]. Together with other parts of the application, SR-Site is currently being reviewed by the Swedish Radiation Safety Authority (SSM). The main method for review of SKB's licensing documentation is document review carried out by SSM, supported by SSM's external experts. However, SSM's document review is also supported by regulatory modeling, technical reviews of SKB's quality assurance program and consideration of external review comments from two broad national consultations and an international peer review organized by OECD's Nuclear Energy Agency [2]. SSM's review is divided into three main phases: the initial review phase, the main review phase and the reporting phase [3].

The overall goal of the Initial Review Phase was to achieve a broad coverage of SR-Site and its supporting references and, in particular, to identify the need for complementary information and clarifications to be provided by SKB, as well as to identify critical review issues that require a more comprehensive treatment in the main review phase. SSM completed the initial review phase in the end of 2012. The on-going main review phase involves in-depth review of the safety critical issues identified in the initial review phase, with the aim of resolving review issues in preparation for a regulatory review statement. A number of review workshops have been held or will be held focusing on various issues. The purpose of the workshops is to have frequent interactions between SSM's consultants and SSM's staff so that multi-disciplinary issues can be discussed. The final reporting is expected during 2015.

SSM and its predecessors have, for several decades, been developing independent models to support regulatory reviews. Modeling teams have been established, combining both in-house and external expertise. SSM's independent modeling can be referred to as one of the following three categories: 1) Use of simple scoping calculations, 2) Use of SKB's own models (with other equation solvers), or 3) Use of alternative conceptual models. Simple scoping calculations may be used to check the reasonableness of SKB's modeling results and to check the impact of individual process descriptions or parameters on radiological consequences. By replicating SKB's calculations with their own models or SSM's interpretations thereof, SSM can gain insight into the details of SKB's calculations that cannot be attained by just reviewing SKB's modeling reports. Finally, the use of alternative conceptual models provides a means to explore different types of uncertainty related to safety critical review issues. In this paper we focus on the independent modeling applied to the consequence analysis part of SR-Site.

Because the KBS-3 method relies heavily on the containment safety function, canister integrity is in the focus of the safety case. In SR-Site, there are two scenarios for which canister failures are not excluded, namely the scenarios 'canister failure due to corrosion' and 'canister failure due to shear load' [1]. Hereafter these two scenarios are referred to as the corrosion scenario and shear load scenario.

SKB'S MODELS FOR THE CONSEQUENCE ANALYSIS

SKB's modeling chain for consequence analysis is shown in Fig. 1. The consequence analysis in SR-Site is based on models which describe radionuclide transport in the near-field, far-field and biosphere. Radionuclide transport in the near-field is modelled with the compartment model COMP23, [4, 5] that models processes related to radionuclide release and transport in the canister interior, the bentonite buffer and in the deposition tunnel backfill. SKB's far-field transport is modelled with FARF31, a one-dimensional advection-dispersion model with matrix diffusion and sorption to describe groundwater radionuclide transport in fractured rock [5, 6]. Dose assessment is performed by a complex model, the so-called Radionuclide Model [7] that describes the continuous development in time of both terrestrial and aquatic biosphere objects, to derive Landscape Dose conversion Factors (LDFs). LDF is defined as the annual effective dose to a representative individual resulting from a constant unit release rate. Doses for any given scenario are estimated by multiplying the LDF values with modelled release rates from the geosphere.

RESULTS OF THE INDEPENDENT MODELING ACTIVITIES

Initial Review of SR-Site

SSM's independent modeling in the initial review phase is an interpretation of the models that SKB utilizes in SR-Site; the numerical software Ecolego [8] is used. Ecolego is a compartment modeling software in which the COMP23 near-field transport model and the Radionuclide Model for dose assessment is implemented. The discretization method proposed by Broed and Xu [9] is used to implement the FARF31 model in the Ecolego. Both deterministic and probabilistic radionuclide release and transport calculations for SKB's corrosion and shear load scenarios, including LDF-values, are reproduced.

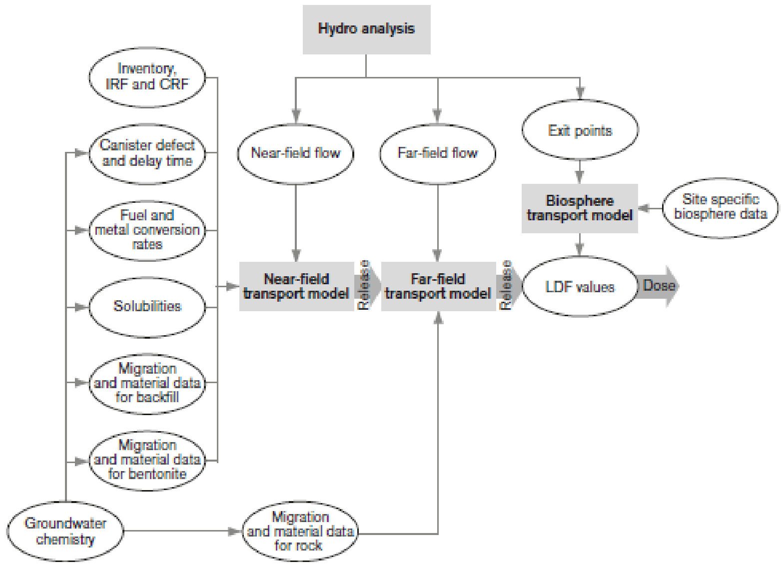

Fig. 1 SKB's models and data for the consequence calculations [1].

Although there was an observed lack of clarity in the model descriptions and the input data used for SKB's calculations, it was possible to reproduce SKB's calculations with certain assumptions. Using the models and input data adopted by SKB, the reproduced results for the corrosion and shear load scenarios as well as the LDF values, are shown in Fig. 2 - 3 and Table A-I in Appendix A. As can be seen, the results from the independent modeling and SKB's calculations are comparable. Similar results were obtained by SSM's consultants, Pensado and Mohanty [10], who used an alternative compartmental representation of SKB's near-field and far-field release and transport models to evaluate SKB's results for the corrosion and shear load scenarios. However, we should bear in mind that at this stage we have not evaluated, for instance, the probabilities of the scenarios, the input data, assumptions and supporting models.

The independent modeling performed during the initial review phase allowed us to get insight into SKB's calculations presented in SR-Site. A number of requests for clarification and complementary information were sent to SKB based on the findings gained from our reproduction of SKB's calculations [11]. These requests concern issues like inconsistency between the documents and the actual modeling performed in SKB's dose assessment, QA problems in the consequence analysis, and insufficient justification of assumptions. Further, a number of review issues and new modeling assignments were identified for the main review phase. The review issues include justification of input data such as K_d values and SKB's methodology for parameterization of flow rates used in the biosphere Radionuclide Model. New modeling assignments include calculations with simple reference biosphere models for comparison with

SKB's complex biosphere model, reproduction of selected "what if" and "residual" scenarios as well as "barrier function" scenarios.

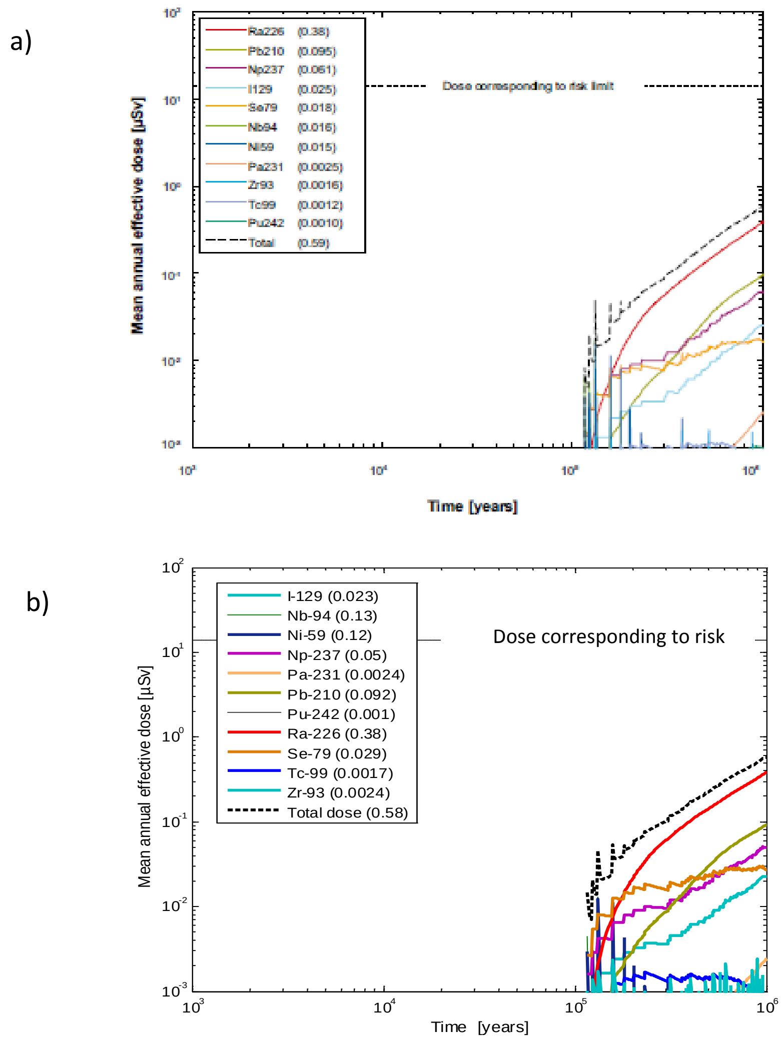

Fig. 2 Near-field dose equivalent release for a probabilistic calculation of the central corrosion scenario. The average number of failed canisters is 0.12. The values in parentheses are peak dose over one million years in units of □Sv, a) is from SR-Site calculation [1,5], b) is SSM's reproduced results.

Main Review of SR-Site

As mentioned earlier the main review phase is ongoing. In the following we present some preliminary results from independent modeling activities, including reproduction of the mean number of failed canisters in the corrosion and shear load scenarios and calculations with alternative simple reference biosphere models.

Reproduction of SKB's mean number of failed canisters in the corrosion scenario

The mean number of failed canisters is essential for the consequence analysis. Requests for clarification and complementary information were sent to SKB in order to have a thorough understanding of SKB's calculations for canister failure due to corrosion. According to the clarification from SKB [12], the mean number of failed canisters due to corrosion under advective conditions (in case buffer is eroded) within one million years is calculated based on all the

a)

b)

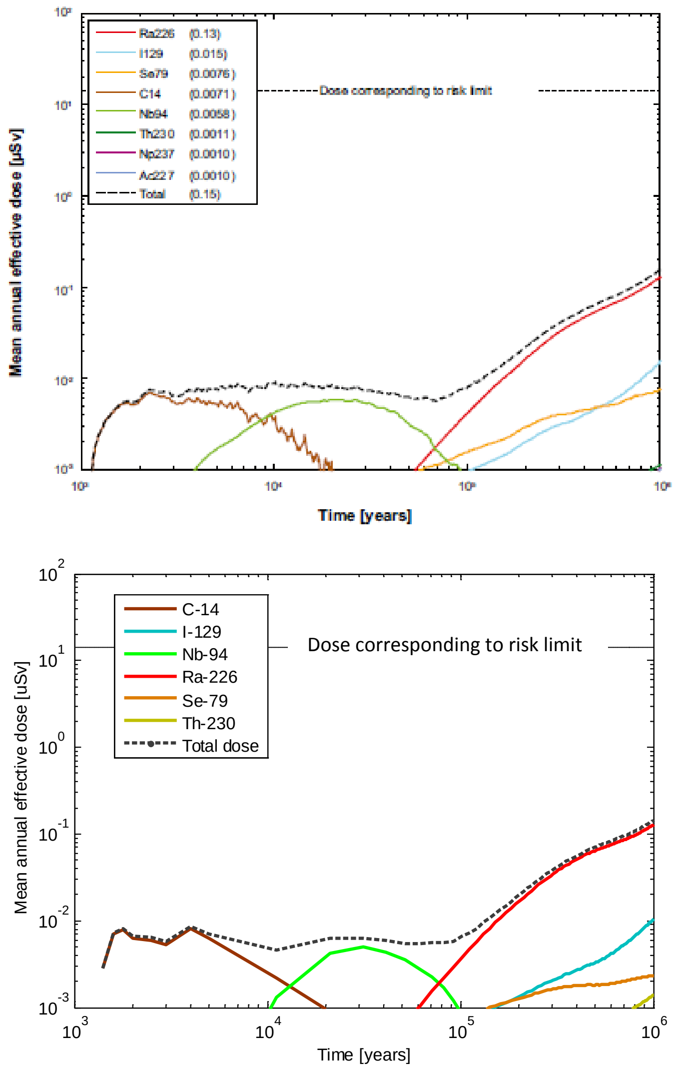

Fig. 3 Near-field and far-field mean annual effective dose for the probabilistic calculation of the shear load scenario, a) is from SR-Site calculation [1, 5], b) is SSM's reproduced results.

combinations of two discrete data distributions: 1) the 6 000 deposition positions with individual equivalent flow rates, Q_{eq} calculated from flow modeling and 2) the 46 sulphide concentrations measured in the groundwater of the Forsmark site, [HS^-]. The time of a canister failure is the sum of the time to reach advective condition, t_{adv}, and the time required to corrode through a canister wall, t_{corr}. The models to calculate t_{adv} and t_{corr} are given below according to the complementary information supplied by SKB [13]:

$$t_{adv} = \frac{m_{buffadv}}{R_{Erosion} \cdot f_{tdilute}} \qquad \text{(Eq. 1)}$$

$$t_{corr} = \frac{d_{Can}}{V_{corr}} = \frac{d_{Can} \cdot A_{corr}}{Q_{eq} \cdot [HS^-]} \frac{\rho_{Cu}}{f_{HS} \cdot M_{Cu}} \qquad \text{(Eq. 2)}$$

in which $m_{buffadv}$ is the amount of buffer mass loss required to reach advective conditions, $f_{tdilute}$ is the fraction of time with groundwater sufficiently dilute for erosion, $R_{Erosion}$ is the erosion rate, d_{Can} is the thickness of canister wall, V_{corr} is the rate of corrosion once advective conditions are reached in the buffer, A_{corr} is the area exposed to corrosion, ρ_{Cu} is the density of copper, Q_{eq} is the equivalent flow rate, [HS^-] is the sulphide concentration, f_{HS} is a stoichiometric factor taking into account the reaction of sulphide with copper, and M_{Cu} is the molar mass of copper.

Reproduction of the number of canister failures was performed by selecting the calculation case of realization r3 of the semi-correlated hydrogeological DFN model. In the calculation the sulphide concentrations are found in Tullborg et al. [14] (see Fig. 4) and equivalent flow rate data were requested from SKB. Other parameter values used in Eq. (1) and (2) are found in the corrosion report [15]. Based on above mentioned information calculated t_{corr} are in agreement with SKB's calculations (see Table I). As can be seen, four sulphide concentrations led to canister failure in the deposition hole ID 2026 (the probability is 4/46) while the highest sulphide concentration led to canister failure in four additional deposition holes (the probability is 1/46 for each deposition position). Finally the number of canister failures for the realization r3 is calculated as 4/46+1/46+1/46+1/46+1/46=0.17.

A question is raised here: Is this discrete distribution method appropriate? Further calculations were performed by the use of random sampling of a continuous distribution function which represents the measured sulphide concentrations to derive the time of canister failure due to corrosion. Over 40 types of Probability Density Functions (PDFs) were fitted and tested against the measured sulphide data. The distribution parameters were fitted to the data by the maximum likelihood method. For each PDF, the goodness of the fit was then tested with the Kolmogorov Smirnov method. The Log Normal distribution with fitted parameters (GM=$1.35 \cdot 10^{-6}$, GSD=4.19) and Inverse-Gaussian distribution (see Fig. 5) with parameters ($\mu = 5.18 \cdot 10^{-6}$, $\lambda = 7.22 \cdot 10^{-7}$) had similar estimated goodness-of-fit properties and were both considered to have a good fit to the data (the p-values associated with the test-statistic >0.8). Probabilistic calculations to estimate the number of canister failures due to corrosion for realization r3 was performed by using Latin Hypercube method with 10 000 samplings based on the above mentioned two distribution functions. The obtained number of canister failures was 0.2 based on Inverse-Gaussian distribution and 0.14 based on Log Normal distribution, respectively. It might be concluded that SKB's method based on the existing data set does not lead to an underestimation of the number of failed canisters.

The above calculations focused on the understanding of SKB's methodology of corrosion calculation. However, further in-depth review of the parameters such as Q_{eq}, $[HS^-]$ and A_{corr} are underway to evaluate if these parameters are reasonably derived because they have a significant impact on the calculated time of canister failure.

TABLE I. Comparison of calculated time for canister failure due to sulphide induced corrosion for 5 canister positions in realization r3 of the semi-correlated hydrogeological DFN model. The possible failures are sorted with the earliest time on top.

Dep. Hole in DFN hydro model	Flow-rate [m^3/yr]	Sulphide conc. [M]	SKB's calculated tcorr [yr]	SSM's calculated tcorr [yr]	Relative error of two calculations
2026	0.251	0.00012	75,216	75,214	0.0%
400	0.079	0.00012	199,919	200,027	0.4%
399	0.06	0.00012	264,285	264,462	0.1%
398	0.047	0.00012	338,906	337,611	0.1%
401	0.042	0.00012	374,632	377,803	0.8%
2026	0.251	1.22E-05	740,617	739,806	0.1%
2026	0.251	1.15E-05	786,905	784,838	0.3%
2026	0.251	1.06E-05	851,709	851,477	0.0%

Reproduction of SKB's mean number of failed canisters in the shear load scenario

To support discussions and identify issues for in-depth review at an earthquake workshop, we reproduced SKB's calculations of the mean number of failed canisters due to the shear load scenario. The frequency of canister failures due to earthquake-induced shear load is shown in Fig. 6 [1]. The area under the graph in Fig. 6 yields the mean number of failed canisters at one million years as 0.079, which is calculated by the two models, equation (3) and (4) [1], to describe the areas of a light blue rectangle and a white triangle, respectively.

$$N_{failed} = 5 \cdot f \cdot t \cdot N_{crit} \qquad \text{(Eq. 3)}$$

$$N_{failed} = \frac{1}{2} \cdot (5 \cdot f)^2 \cdot \left(10^6 - T\right)^2 \cdot N_{crit,2nd} \qquad \text{(Eq. 4)}$$

in which N_{failed} is the number of canisters that may fail, f is yearly frequency of earthquakes ≥M5 within a 5 km radius area, t is the time, T is the relaxation time, and N_{crit} and $N_{crit,2nd}$ are the average number of canisters in critical position.

Three parameters, f, N_{crit} and $N_{crit,2nd}$ have significant impacts on the calculated number of failed canisters at one million years. However, the values of these three parameters are derived through a number of steps including various process descriptions, modeling and approaches. By inserting the parameter values given in [1] into Eq. (3) and (4), we have calculated the mean number of failed canisters at one million years (the sum of Eq. (3) and (4)) to be 0.074. When using the value of N_{crit} from Munier [16], the calculated value is 0.078 which is closer to the SKB's value. This calculation was presented at the earthquake workshop and the detailed processes behind these three parameters were discussed. Some new review issues were identified during the workshop that will lead to new assignments for the in-depth review.

Comparison between simple reference biosphere models and SKB's complex biosphere model

The complex biosphere model, Radionuclide Model, was developed by SKB for the biosphere dose assessment in the SR-Site [7]. The Radionuclide Model is built on a landscape evolution model, whereby radionuclide releases to distinct hydrological basins/sub-catchments (termed 'objects') are represented as they evolve through land rise and climate change. The output from the Radionuclide Model is LDF values as mentioned earlier. The Forsmark site is located on the Baltic coast with a terrestrial landscape including lakes, mires, forest and arable land. The land at

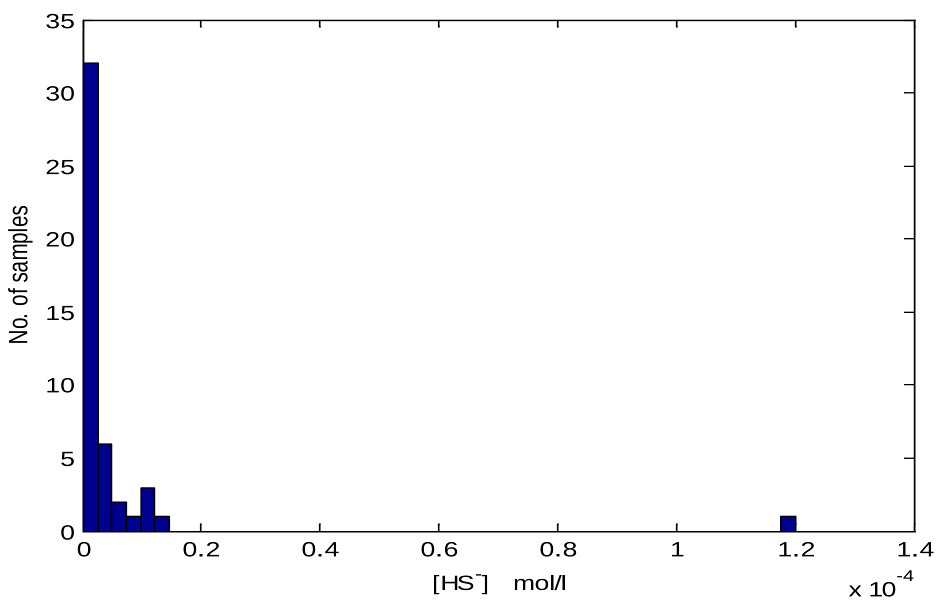

Fig. 4 Histogram of measured sulphide concentration in the groundwater at the Forsmark site.

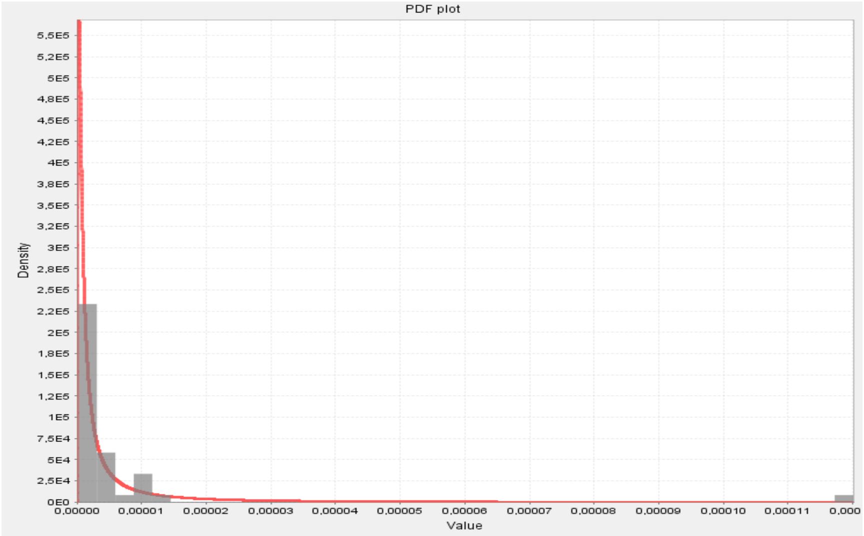

Fig. 5 Inverse-Gaussian distribution (solid line) fitted to the measured sulphide data with parameters (μ=5.18·10^{-6}, λ=7.22·10^{-7}).

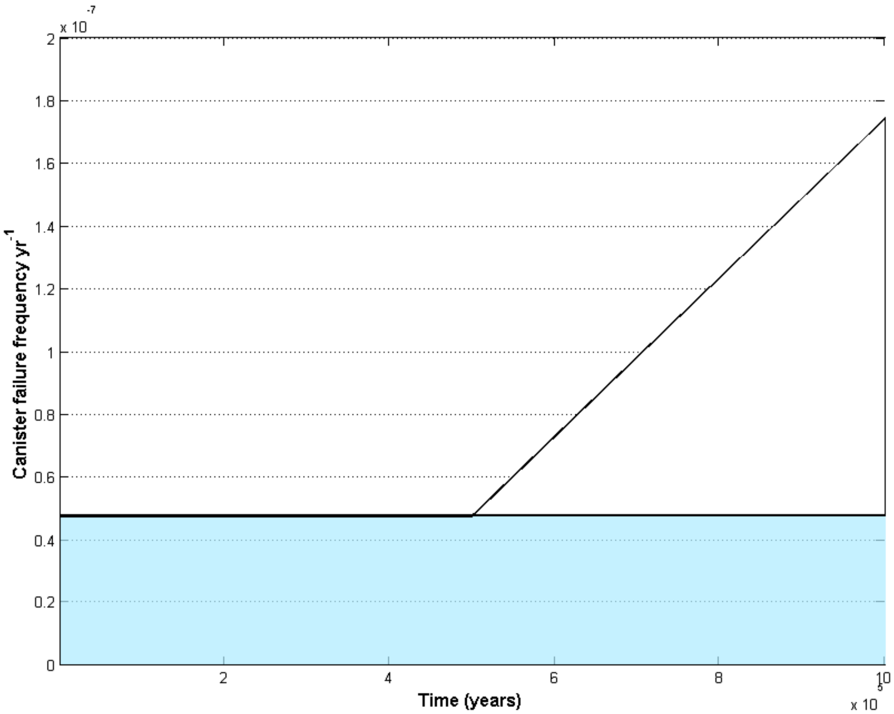

Fig. 6 Frequency of canister failures due to earthquake-induced shear load as a function of time (after SKB [1] with minor modifications).

the site is projected to continue to rise due to post-glacial uplift leading to ecosystem transitions in excess of ten thousand years. Owing to the complexity of the approach adopted by SKB in the biosphere dose assessment, it is difficult to penetrate all the details through document review only. Therefore SSM's review method includes 1) reproduction of SKB's LDF values (see previous section) to get insight into the methodology used in SR-Site and 2) performance of calculations with alternative models to explore conceptual model uncertainty in support SSM's final compliance judgments.

Simplified reference biosphere models were developed to represent the most plausible transport processes and various types of 'objects' such as a well, agricultural land, lake and wetland [17]. The output from these simplified models is a set of dose conversion factors for various types of 'biosphere objects' resulting from a constant unit release rate. The models draw on the data used in SR-Site as much as possible to help ensure meaningful comparison of the results with SKB's results. However, the simpler models do not include an explicit representation of the succession between different biosphere systems (e.g. succession from marine to lake to mire to terrestrial systems) and changes of 'object' size with time. The area considered for the simple biosphere models were derived independently of the biosphere 'object' approach adopted in SR-Site (see Table II).

Comparison of the SR-Site LDFs with equivalent dose conversion factors calculated with the simple biosphere models show that:

- for most radionuclides, the explicit representation of transitions between marine, lake, mire and terrestrial systems results in dose factors that are more than one order of magnitude greater than those calculated with simple, non-evolving biosphere systems;
- for six radionuclides, the simple biosphere models resulted in dose factors more than an order of magnitude higher than those used in SR-Site when equivalent assumptions were adopted; and
- SKB's focus on exposure of adults in SR-Site is generally justified, but it should be borne in mind that doses to children and infants could be up to a factor of seven higher for certain radionuclides.

Potential exposures arising from assumptions such as the use of shallow wells for small-scale horticulture in addition to domestic and other agricultural uses and the consideration of dose from child and infants result in dose factors that are higher than those considered in SR-Site for some radionuclides for which comparison was possible. These uncertainties will be further explored in SSM's main review phase.

TABLE II. The area considered for simple biosphere models

Object	**Marine**	**Lake**	**Mire**	**Forest**	**Pasture**	**Arable**
Area (m^2)	2,000,000	50,000	50,000	50,000	100,000	10,000

CONCLUSIONS

Reproduction of radiological consequences for corrosion and shear load scenarios as well as LDF values has been carried out in the initial review phase. The findings obtained through the reproduction of SKB's calculations have helped us to identify critical issues for in-depth review as well as a number of requests for clarification and complementary information. Requests of clarification and complementary information include issues regarding inconsistency between the documents and the actual modeling performed in SKB's dose assessment, QA problems in the consequence analysis, and insufficient justification of assumptions.

SSM communicated the results from the initial review phase on the 29th October 2012 by handing in a written statement to the Land and Environment Court and SKB [18]. SKB has also been informed about the results of SSM's independent modeling through SSM's request for complementary information.

In the main review phase, reproduction of calculations of the mean number of canister failures for two scenarios has so far been completed. A number of parameters, processes and assumptions which have significant impact on the calculated results have been identified and are to be further evaluated in the main review phase. By the use of alternative simple biosphere models we were able to evaluate process uncertainty and check the reasonableness of SKB's complex, and not always that transparent, biosphere model. The findings from this model comparison suggest that LDF values are generally not underestimated for important radionuclides in SR-Site for releases to surface soils/sediments via groundwater.

SSM's independent modeling has enabled detailed insight into SKB's consequence analysis in the SR-Site safety assessment that could not have been attained by review of modeling reports alone. Before coming to our final conclusions on SKB's consequence analysis, a number of reviews and modeling assignments remain. More requests for clarification and complementary information cannot be excluded.

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APPENDIX A RESULTS OF THE COMPARISON OF TWO CALCULATIONS: SKB'S SR-SITE LDFS AND SSM REPRODUCTION

TABLE A-I. A comparison of the simulated LDFs with SKB's LDFs for biosphere object 121_03.

Radionuclides	SSM's calculations	SKB's calculations	Ratio of two calculations
	LDF [Sv/y per Bq/y]	LDF [Sv/y per Bq/y]	
Ac-227	8.00E-12	8.00E-12	1
Am-241	1.51E-12	1.50E-12	1.01
Am-243	1.53E-12	1.50E-12	1.02
Ca-41	7.85E-14	9.90E-14	0.79
Cl-36	7.85E-13	5.80E-13	1.35
Cm-244	8.73E-13	8.70E-13	1
Cm-245	1.62E-12	1.60E-12	1.01
Cm-246	1.56E-12	1.60E-12	0.98
Cs-137	1.01E-13	1.20E-13	0.84
I-129	4.07E-10	6.50E-10	0.63
Ni-59	1.57E-13	7.40E-14	2.12
Ni-63	1.18E-15	1.20E-15	0.98
Pa-231	1.34E-11	8.10E-12	1.65
Pb-210	2.61E-11	5.10E-12	5.12
Pd-107	9.68E-15	6.70E-15	1.44
Po-210	8.87E-12	8.90E-12	1
Pu-239	2.02E-12	1.90E-12	1.06
Pu-240	1.89E-12	1.90E-12	0.99
Pu-242	1.96E-12	1.90E-12	1.03
Ra-226	2.20E-11	3.80E-12	5.79
Se-79	1.24E-09	1.20E-09	1.03
Sm-151	7.14E-16	7.20E-16	0.99
Sn-126	9.81E-12	2.50E-11	0.39
Sr-90	2.09E-13	2.20E-13	0.95
Th-229	6.67E-12	3.60E-12	1.85
Th-230	1.85E-12	1.30E-11	0.14
Th-232	1.86E-12	1.70E-12	1.09
U-233	5.04E-12	2.50E-12	2.02
U-234	4.78E-12	3.60E-12	1.33
U-235	4.97E-12	2.80E-12	1.78
U-236	4.58E-12	1.90E-12	2.41
U-238	4.38E-12	1.90E-12	2.31
Zr-93	6.41E-14	2.80E-14	2.29