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2015:05

Review of uncertainty propagation and sensitivity analysis in SR-Site

Main Review Phase

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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 och göra expertbedömningar i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Det övergripande syftet med projektet är att ta fram synpunkter på SKB:s säkerhetsanalys SR-Site för den långsiktiga strålsäkerheten hos det planerade slutförvaret i Forsmark. Det specifika syftet med projektet är att (1) granska och bedöma tillämpbarheten av SKB:s metoder för känslighetsanalyser och osäkerhetsanalys i SR-site, (2) bedöma SKB:s ansats för användning av försiktigt valda (konservativa) respektive realistiska parametervärden och antaganden samt (3) att granska SKB:s propagering av osäkerheter i det riskdominerande scenariot med erosion av buffertmaterial i deponeringshål följt av advektiva förhållanden och accelererad korrosion av kopparkapseln.

Författarens sammanfattning

Granskningsuppdraget SSM2014-2060 "Granskning av osäkerhets- och känslighetsanalys i SR-Site" omfattar tre frågor:

1. Tillämpbarhet av SKB:s metoder för genomförande av känslighetsanalyser
2. Metod för användning av konservativa respective realistiska parametervärden
3. Propagering av osäkerheter i korrosionsscenariot

Tillämpbarhet av SKB:s metoder för genomförande av känslighetsanalyser:

Känslighetsanalyser genomfördes med väletablerade metoder och valet av metoder har motiverats på ett bra sätt. De valda metoderna förefaller lämpliga och resultaten är rimliga och dessutom understödda av fenomenologiska resonemang kring fysiska och kemiska processer. Granskaren menar att ytterligare systemförståelse hade kunnat uppnås om känslighetsanalyser genomförts inte bara för dosberäkningarna utan även för beräkningar av säkerhetsfunktionsindikatorer. I rapporten ger granskaren förslag angående hanteringen av sinsemellan beroende indata.

Försiktigt valda (konservativa) respektive realistiska parametervärden:
SKB hanterade parameterosäkerheter antingen genom att ange en sannolikhetsfördelning eller genom att ansätta försiktigt valda parametervärden (undantag: parametrar som användes för biosfärsberäkningar). Säkerhetsanalysen SR-Site befinner sig följdaktligen i den (ganska vanliga) situationen att den resulterar i "pessimistiska skattningar av osäkerhet", d.v.s. den resulterar i fördelningar som är förskjutna åt det pessimistiska hållet (och sannolikt också med en ändrad fördelningsform). Detta är lämpligt vid bedömning av kravuppfyllelse, men det innebär också att slutsatser om känsligheter behöver analyseras och testas ytterligare innan de kan användas för att bestämma behov av ytterligare forskning och utveckling.

Propagering av osäkerheter:
Utöver den deterministiska hanteringen av många osäkerheter, hanterades flera avgörande osäkerheter för bufferterosion och kapselkorrosion med probabilistiska metoder. Olika metoder användes i argumentationen för att kapselbrott endast sker i samband med bufferterosion och för att härleda indata till konsekvensberäkningar oc h risksummering för detta fall. Det är viktigt att skilja på (i) epistemiska osäkerheter kopplade till sprickfördelningen och den resulterande grundvattenflödesfördelningen och (ii) den rumsliga fördelning för båda. För den förra finns det två nivåer: (ia) den okända korrelationen mellan transmissivitet och sprickstorlek och (ib) den verkliga sprickfördelningen som är okänd men som ska täckas in av de olika realiseringarna av den diskreta spricknätverksmodellen för de olika korrelationsmodellerna. Dessutom är den (osäkra) rumsliga fördelningen och temporala utvecklingen av sulfidkoncentrationer betydelsefull. Dessa kategorier hanterades av SKB men argumentationen är till viss del baserad på en sammanblandning av rumslig och temporal variabilitet med epistemisk osäkerhet och på ett implicit antagande om stationära förhållanden som varken diskuteras eller motiveras. Granskaren anser att det är mycket troligt att konsekvenserna överskattades med SKB's konservativa ansats men en strikt förklaring och motivering saknas på visa ställen.

Projektinformation
Kontaktperson på SSM: Björn Dverstorp
Diarienummer: SSM2014-2060
Aktivitetsnummer: 3030012-4115

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 and provide expert opinion on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

The general objective of the project is to provide review comments on SKB's postclosure safety analysis, SR-Site, for the proposed repository at Forsmark. The specific objectives are (1) to review and assess the suitability of SKB's methods for sensitivity and uncertainty analyses, (2) to review SKB's approach for use of conservative and best-estimate parameter values, and (3) to review SKB's propagation of uncertainty in the main risk-driving scenario in SR-Site with buffer erosion leading to advective conditions and enhanced copper corrosion.

Summary by the author

The review assignment SSM2014-2060 "Review of uncertainty and sensitivity analysis in SR-Site" addressed three issues:

1. Adequacy of the methods adopted by SKB for conducting sensitivity analyses
2. Approach for use of conservative and best-estimate parameter values
3. Propagation of uncertainty for the corrosion scenario

Adequacy of the methods for sensitivity analyses:

The sensitivity analyses (SA) were carried out using well-established approaches the choice of which is adequately justified by SKB. The choice of SA methods seems appropriate and the results obtained reasonable and furthermore supported by physico-chemical reasoning. The reviewer wonders whether further insight about system behaviour could have been obtained by carrying out SA not only for the results of dose calculations but also for THMC models used for calculating safety function indicators. Suggestions concerning the handling of dependent inputs were made by the reviewer.

Conservative and best-estimate parameter values:
Parameter uncertainties were treated by SKB either by assigning probability distributions or by assigning values on the cautious side (exception: parameters used for the biosphere calculations). SR-Site is thus in the (rather common) situation that the probabilistic calculations deliver a "pessimistic estimate of uncertainty", i.e. they deliver distributions which are shifted to the pessimistic side (and most likely also changed in shape). This is appropriate for compliance demonstration but it also means that the sensitivity statements have to be further investigated and tested as to their practical relevance before they can transferred into specifications concerning further R&D.

Propagation of uncertainty:
Apart from the deterministic treatment of many uncertainties, there were several uncertainties decisive for buffer erosion and canister corrosion which were handled probabilistically. Different approaches were used when arguing that canister failure can only occur in the case of buffer erosion and when deriving the input for the consequence calculations and risk summation in such a case (of buffer erosion). One has to distinguish between (i) (epistemic) uncertainty about the fracture distribution and resulting flow field and (ii) the spatial variability of both. For the former, there are two levels: (ia) the unknown correlation between transmissivity and fracture size and (ib) the in-situ fracture distribution which is unknown but should be covered by the range of discrete fracture network (DFN) realisations for the various correlation models. Furthermore, the (uncertain) spatial distribution and temporal evolution of sulphide concentrations are of importance. These categories were addressed but the argumentation is to some extent based on a confusion of spatial and temporal variability with epistemic uncertainty and on implicitly using a stationarity assumption which is neither discussed nor substantiated. The reviewer considers it very likely that consequences were overestimated by applying SKB's conservative approach but a strict explanation and justification is lacking at some places.

Project information
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Contents

1. Introduction

This report covers Parts 1 and 2 of the review assignment SSM2014-2060 “Review of uncertainty and sensitivity analysis in SR-Site”.

Part 1 addresses the issues

- adequacy of the methods adopted by SKB for conducting sensitivity analyses

and

- adequacy of the methods adopted by SKB for quantifying uncertainty.

According to the specification of work this includes

- adequacy of SKB’s methods for sensitivity analysis given their use in SR-Site,
- SKB’s justification of their methods for sensitivity analysis, including the potential for using other methods to improve understanding about critical parameters,
- approach for use of conservative and best-estimate parameter values and
- assumptions account of relevant review comments given on the SR-Can safety assessment.

In chapters 2 and 3, the report presents the authors’ assessment in response to these questions raised by SSM.

Part 2 of the review assignment comprises a review of the propagation of uncertainty in the buffer erosion / canister corrosion scenario (hereinafter briefly called “corrosion scenario)”, which contributes most to the risk calculated by SKB. At a meeting held in October 2014 it was agreed with SSM that the focus should be on the ways several types of uncertainties were characterised and propagated via the determination of the canister failure distribution to the risk calculation (chapter 4).

2. Adequacy of the methods adopted by SKB for conducting sensitivity analyses

2.1. Motivation of the assessment

Since decades, sensitivity analyses (SA) of one or the other kind form part of performance assessments, safety assessments, and safety cases for deep disposal of radioactive waste. Traditionally, the term "sensitivity analysis" refers to analysing the relationship between inputs and outputs of model calculations. In the broadest sense, the term "input" might include the choice of model assumptions (possibly including the postulation of scenarios), of calculation models / computer codes (which of course also includes a choice concerning model assumptions), and numerical input parameters for model calculations.

Analyses of choices concerning scenarios, model assumptions, calculation models and computer codes are usually being done by simply deterministically testing one choice against the other, ideally in a thorough, comprehensive and systematic way. In the SR-Site Main Report (SKB, 2011), such testing activities are being reported at several places, including sections 10.3.5, 10.3.6, 10.3.8, 10.3.12, 10.4.5 (here with explicit mention of the term "sensitivity analysis"), 10.4.6., 12.2.2 (again with mention of "sensitivity analysis"), 12.3.2 ("sensitivity study", "sensitivity tests"), 12.6.2 ("Quantitative sensitivity analysis"), 13.2.4, and 13.5.6. The overall approaches for doing this are described in sections 2.5 and 2.8 (in particular 2.8.3) of SR-Site. The author believes that such handling of uncertainties as described in section 2.8.3 under the headings "Scenario selection", "Conceptual uncertainty", and "Modelling" is of utmost importance for any safety assessment and crucial for understanding what uncertainties exist and what the consequence of their existence for achieving and assessing long-term safety is. He even believes that in many cases these uncertainties are much more important than uncertainties concerning input data of calculation models.

Nevertheless, the author's understanding of his assignment is that SKB's handling of scenarios and conceptual uncertainties is being addressed elsewhere in SSM's review framework, cf. e.g. Wilmot (2012). Therefore, this note focusses on the issue of SA in the narrower sense, i.e. on the investigation of the relationship between input and output data of model calculations. Even in this narrower sense, there is variety of interpretations of the word "sensitivity analysis", see e.g. Becker et al. (2009), Bolado-Lavín et al. (2008), and Kuhlmann et al (2013). The perhaps most important distinction to make is the one between methods which address the response of model outputs to inputs with given uncertainties (described by probability distributions of these inputs) and methods which address only the model itself without accounting for input distributions. Especially for the former, there exists a wide variety of mathematical / numerical methods, some of them being rather sophisticated. Dependent on the method used, the analysis can address different types of input-output relationships, e.g. linear, monotonic (including non-linear monotonic), non-monotonic, impact on the output probability distribution. The analysis might not only address the impact of single input parameters, but also the combined influence of two or even more parameters ("interactions"). Ongoing research strives for improvement and development of such methods.

Kuhlmann et al (2013) however report that most of these methods are not being used in safety assessments for radioactive waste disposal. They further suggest that this fact in itself does not necessarily mean that these assessments have deficiencies. However, they also suggest that a comprehensive SA should not only report the calculated sensitivity measures for the single input parameters but should also address the question to which extent these measures explain the model behaviour (e.g. by reporting the coefficient of determination R^2 for regression analyses). The author of this note, being also a co-author of (Kuhlmann, 2013), shares this view. Kuhlmann et al. (2013) further provide a sketch for a methodology of successively applying different methods with the option to stop the analysis once a satisfactory explanation of the model behaviour is obtained. This methodology is however the topic of an ongoing research project and can therefore not (yet?) be considered as state-of-the-art.

With respect to SSM's topic "adequacy of SKB's methods for sensitivity analysis", the review will therefore address the questions

- To which models was the SA applied?
- Did the SA yield results explaining the model behaviour sufficiently well and was this reported by SKB?

2.2. SKB's presentation

2.2.1. SA for the central corrosion case

Sensitivity analysis in the "narrow" sense (i.e. numerical methods to determine relationships between model inputs and outputs, see Introduction) is being presented in section 13.5.11 of SR-Site. The analysis was carried out for the dose calculation model (total and the Ra-226 doses) for the central corrosion case (Section 13.5.4). SKB motivates the choice of Ra-226 by referring to its dominance in most realisations and states that the SA is motivated by learning about "correlations" as well as about identifying parameters which are related to high and low doses. SKB further elaborates about the existence of a variety of SA methods and motivate their choice of SA by standardised rank regression coefficients (SRRC) by the monotonicity of the system. SRR has been carried out for the "total dose at 10^6 years". SKB then names the parameters identified by this analysis: the fuel dissolution rate, the transport resistance along the geosphere flow path, and the canister failure time (descending order). For the Ra-226 dose the SA yielded the transport resistance along the geosphere flow path, the fuel dissolution rate, and the canister failure time. SKB's interpretation of the different order is that the transport resistance is especially important for sorbing nuclides, some realisations being not dominated by Ra-226 but by the non-sorbing I-129. SA for the total dose maximum over time yielded similar results. Apparently, SKB did more SA; in SR-Site it is also referred to SA on the maximum Ni-59 dose and the language suggests that there was even more SA which is, however, not explicitly mentioned or described. In Figure 13-43 of SR-Site, coefficients of determination R^2 of around 0.9 are indicated.

In addition, a conditional mean value analysis was carried out in order to "determine the variables that are related to the highest doses" (the same for low doses as well as for both high and low extreme outcomes). The analysis yielded the failure time, the fuel dissolution rate, the transport resistance and a parameter called t_W for the high values.

SKB mentions that the transport resistance, the failure time and a third parameter t_W are correlated "meaning that their significance is not necessarily as high as indicated by the SRRC method. This was further investigated with a tailored regression model … ."

This model is based upon *a priori* knowledge about the dose calculation model. In this model, regression of the calculated data with a series of four pre-defined approximation models was carried out, starting with a model using just one parameter and stepwise expanding it using a second, then a third, and then a forth parameter. With four parameters, the approximation model explains the original one with an R^2 of 0.99. This leads SKB to the claim "that the variable t_w, identified as important for the Ra-226 dose by the SRRC method above is not needed to explain the Ra-226 dose. It is concluded that t_w is identified in the SRRC method only since it is correlated to the F parameter. (This can be further analysed through use of partial rank correlations in the SRRC method.)"
Finally, SKB presents a scatterplot "showing how high and low dose results relate to the variable groups", but in fact meaning by "variable groups" rather functions of variable groups.

2.2.2. SA for canister failure due to shear load

Again, SKB performed SA by means of SRRC for the same quantities of interest as described above. R^2 values of 0.69 to 0.94 are reported. A physico-chemical discussion of the results obtained is given.

2.3. The Consultants' assessment

SKB's approach to carry out SA (only) for the dose calculation model is a very established and traditional one. Nevertheless, given the high importance of safety function indicators in SKB's methodology, the author wonders whether further insight about system behaviour could have been obtained by carrying out SA also for THMC models used for calculating such indicators.
The data for the probabilistic calculations for the central corrosion case, and thus for the SA, are based on the semi-correlated DFN model. Again, the question arises why the analysis was restricted to this model.
An important conceptual step in SA when calculating time-dependent results is the choice of the "quantity of interest", i.e. the transfer of the calculated time series into one single value for which the SA will be carried out. Since the maximum annual effective dose is decisive for regulatory compliance, it is an obvious choice for such a value. Indeed, SKB decided to perform SA for maximum annual effective doses. In addition, SA for annual effective dose at the end of the calculation timeframe (10^6 years) was performed. Given that the calculated annual effective dose for the deterministic calculation as well as the mean value for the probabilistic calculation is still increasing at this time, this is also an obvious and reasonable choice. Other possible choices would have been the time of maximum or the integral over time, but the reviewer is not sure whether this would have led to additional insight. Some authors also present the evolution in time of sensitivity measures (here: SRRC), but in the opinion of the reviewer the insight one can get from such a presentation is limited, especially for the SKB model. (For more complex models with non-monotonic or threshold behaviour, such a presentation could provide insight about the change of "regimes" over time, but this seems not to be the case for the SKB model.)
SKB's choice of SRRC is based on the *a priori* knowledge about the monotonic model behaviour and is justified by the R^2 values obtained. Perhaps, the additional use of some or the other graphical method would have been illustrative for the reader.

The fact that the canister failure time (one of the parameters identified as sensitive) is treated in a quasi-probabilistic manner (56 failure times each combined with 50 realisations for the transport calculations, see chapter 4.1 below) somewhat spoils the theoretical thoroughness of the approach but is, in the opinion of the reviewer, of no practical consequence.

In summary, the choice of SA methods seems appropriate and the results obtained reasonable and furthermore supported by physico-chemical reasoning. Due to the reasons explained above, this is being said in spite of the advice given by the authorities in their review of the predecessor analysis SR-Can "that SKB should consider other methods apart from the SRRC method ("Standardised Rank Regression Coefficients") to increase the reliability of the results" (Hedin, 2011).

A problem, however, is caused by the fact that that the input parameters are not independent from each other. If there is a relationship between input parameters, the best situation is when this relationship can be explained by physico-chemical reasoning and expressed by a formula which clearly shows a one-way dependency (or perhaps a formula including a random term). If this, as in the SKB case, is not feasible, an approach as taken by SKB (i.e. expressing the relationship by means of a joint parameter distribution, in this case using a correlation) makes sense as long as this joint distribution is justified e.g. by data (as the ones shown in Figure 13-14) – be it measurements or, as in this case, results of process model calculations. This, however, is only true for uncertainty analyses: In uncertainty analyses, in which only the uncertainty of the model output is analysed, this output uncertainty is better characterized when input dependencies are accounted for. The situation is different, though, for SA: Joint probability distributions do not "care" about cause-effect relationships. A joint probability distribution of parameters A and B in which A and B are not independent (e.g. correlated) might be caused by an impact A has on B, or vice versa, or by an impact a third (unknown) C has on both. Which variant is true cannot be seen when looking at the distribution. Therefore, SA in such cases will not be able to separate the effect of A on the result from the effect of B. This is true for the SRRC (as apparently recognized by SKB), but even the application of the tailored regression model will not really improve the situation (despite of SKB's claim): It might well be that another tailored regression model could be found which is based on a partially different set of parameters (some of which correlated to the ones used by SKB) which could then explain the model outcome equally well. Thus, SKB's conclusion on the importance of one of the correlated parameters (and the unimportance of the other one) seems to be based on the *a priori* knowledge the tailored regression model is based on rather than on a reasonable SA outcome.

A promising option to separate an "important" from an "unimportant" parameter when the two are not independent would be to run two SA: One with dependent, the other one with independent parameters, with the same marginal distributions for both.

SKB's application of conditional mean value analysis for identifying parameters important for high, low, and generally extreme values is an interesting and well-justified approach which yielded sensible results.

SKB's conclusion about the possibility of identifying important parameters by relatively simple methods being in part due to the features of the model (buffer omitted, monotonic behaviour) is justified. The physico-chemical interpretation of the results obtained seems to be appropriate.

For the for canister failure due to shear load, the reviewer wonders why SKB did not undertake further investigations for the annual effective doses at 10^6 years for which relatively low R^2 values were obtained. However, the R^2 of .94 for the more interesting maximum value seems to indicate that here the model behaviour was well explained. The physico-chemical discussion of the results seems reasonable.

Finally some remarks about presentation: It was sometimes hard for the reviewer to find the physical entities behind the parameter names. There were also some small mistakes or omissions in the labelling of some figures, but they did not lead to misunderstandings.
The reviewer agrees, also from the viewpoint of SA, with Wilmot (2012) in saying "There are only very limited illustrations of the probabilistic results, with most figures show mean dose. If not included and described in more detail in the underlying reports, a more detailed presentation of such results, which would be useful in understanding the sensitivities to tails of the parameter distributions, should be sought from SKB. "

3. Approach for use of conservative and best-estimate parameter values

3.1. Motivation of the assessment

Uncertainties concerning parameter values in safety assessments, if treated deterministically, can be handled in various ways: “Modelling, especially when aiming at compliance demonstration, might cover complex issues by taking approaches erring on the conservative side. Such conservatism often serves well but its usefulness depends on the stage of repository development and lifecycle. Often, dependent on the purpose of the analysis and on the component to be studied, but especially when options are to be compared for optimisation purposes, moving towards less conservative approaches, which are closer to our understanding of the system and its details, is necessary. ” (OECD/NEA 2012) Such less conservative approaches are sometimes called “realistic” but might be better described as “best guess” or “best estimate” (OECD/NEA 2012).
In cases in which the use of conservative choices is mixed with the use of best estimates and / or probabilistic approaches, the question about the meaning of the results arises. The ensuing sections address this issue.

3.2. SKB’s presentation

Section 2.5.6 (SKB, 2011) about the compilation of data points to section 9 of the same report. There, the following points are made:

- Necessity of a methodology to address input data and their uncertainties
- Data report with the function to compile input data with uncertainty estimates
- Use of standardised procedures
- Distinguish between judgments by “data suppliers” from those made by assessment team
- QA measures, e.g. specific instruction on “Supplying data for the SR-Site Data report”
- Identification of data “uncertain to an extent critical to the safety evaluation, thus requiring a detailed quantification of uncertainty. These data are identified by sensitivity analyses of calculation results using preliminary input data ranges, often from earlier assessments”
- Data qualification in a standardised sequence of stages
- Supplier’s data qualification in the form of probability distributions or, if not possible, “a range. However, the meaning of the range has to be provided, e.g. does it represent all possible values, all “realistically possible” values or just the more likely values? … If it is impossible to express the uncertainty by means other than a selection of alternative data sets or by pessimistic assumptions, this is allowed, as long as the supplier clearly documents this together with the motivation for adopting this approach.”
- Judgement by the SR-Can team (“customer”) with the option to suggest probability distributions

In section 2.8.1 it is said that "…there are several conceivable strategies for deriving input data. One possibility is to strive for pessimistic data in order to obtain an upper bound on consequences in compliance calculations. Another option is the full implementation of a probabilistic assessment requiring input data in the form of probability distributions." Again, reference is made to section 9 as well as to the data report.

In the SR-Site Main Report (SKB, 2011), the choice of pessimistic assumptions or data is mentioned at several places, mostly in connection with a justification based on phenomenology and/or modelling.

3.3. The Consultants' assessment

It is striking that the word "conservative" is not being used in (SKB, 2011) in the sense it is used by SSM in the review assignment. At several place "pessimistic assumptions" are mentioned, though (not only in relationship to data, but also to likelihoods of occurrence / scenario probabilities).

Language as quoted above suggests that there was a high preference for getting probability distributions or at least ranges (with qualifications about the meaning of these ranges) when *supplying* data. It also suggests that pessimistic data should only be supplied in exceptional cases.

The situation is apparently different at the side of the "*customer*" (i.e. the assessors in the SR-Site team). He uses pessimistic assumptions for data at various places, many of them not directly connected with the dose modelling, but rather in considerations and models which formed the basis for the dose models. The reviewer is not in a position to judge about all the individual justifications for such choices but comes to the conclusions that, if these conclusions are sound, the data uncertainties are sometimes addressed by means of probability distributions and in other cases by pessimistic assumptions in the overall modelling framework. The reviewer has not the impression that fixing parameters as best estimates played a role in the probabilistic calculations.

In other words: Many if not all probabilistic calculations carried out by SKB are based on assigning probability distributions to some parameters and fixed values to others. If fixed values were chosen, this has been done pessimistically (if the single justifications are correct). Pessimistic assumptions also played a role in the considerations and modelling work preceding, underlying and "feeding" the dose calculations. The only exception seems to be the biosphere modelling: While the reviewer has not the expertise to judge about the details of this part of the assessment, he still got the impression that the biosphere modelling is based on "best estimate" rather than conservative assumptions.

SR-Site is thus in the (rather common) situation that the probabilistic calculations deliver a "pessimistic estimate of uncertainty". This means that if there were "real" or "correct" distributions of the results, then the calculations do not deliver these "real" distributions but others which are shifted to the pessimistic side (and most likely also changed in shape). Since SKB apparently did not use best estimates for fixing parameters, this is good enough for compliance demonstration. The treatment of the biosphere model (see above) is not necessarily in contradiction to this finding since the biosphere model can be seen as a means to judge the consequences of calculated (uncertain) nuclide releases by multiplying these releases with the Landscape Dose conversion Factors (LDFs) obtained with the biosphere model. Thus, uncertainties related to the biosphere are different in nature from uncertainties related to the repository's containment capability. In the opinion of the reviewer this approach is still justified as long as it is agreed that SKB's calculation results are “not be regarded as measures of health detriment” but rather” represent indicators of the protection afforded by the disposal system” (ICRP 2007, 2013).

However, the uncertainty and sensitivity statements derived from the results always refer to the (pessimistic) model rather than to the system itself. This is an unfortunate situation not only for SR-Site but for most if not all probabilistic uncertainty and sensitivity analyses for deep radioactive waste disposal. At current, there is no conceptual answer to this point. It implies, that particularly sensitivity statements have to “taken with a grain of salt”, i.e. have to be further investigated and tested as to their practical relevance before they can transferred into specifications concerning further R&D. Such an investigation should not only address the pessimistic choices mentioned above, but also all other model assumptions and choices.

The reviewer recommends that SKB explains upfront the strategy used by the “customers” (assessors) when deciding which uncertainties are treated probabilistically and which deterministically / pessimistically.

4. Propagation of uncertainty for the corrosion scenario

4.1. Motivation of the assessment

SSM's regulation requires, amongst many other things, that the implementer presents estimates of the risk resulting from the repository. SKB addresses this requirement by calculating mean values of the probability distributions calculated for the annual effective dose using the probabilistic approach as discussed above. Therefore, the probability distributions underlying these calculations are decisive for the results. In particular, the probability for canister failure is needed for deriving risk values since only such failure could lead to radiological consequences. In the following, the way SKB derived probability distributions for the main risk contributor, the scenario in which an eroded buffer leads to copper corrosion rates sufficient to penetrate the canister ("corrosion scenario") is addressed.

4.2. SKB's presentation

When addressing canister failure by copper corrosion, most of the technological and phenomenological uncertainties associated with buffer erosion and canister corrosion are discussed in the SR-Site Main Report (SKB, 2011) based on information from the various process, data, climate, and / or production / construction reports. However, for understanding the way canister corrosion rates were estimated by SKB, it was also necessary to study the Corrosion Calculations Report (in the Main Report (SKB, 2011) referred to as /SKB 2010d/, hereinafter as (SKB, 2010a)).

Based on FEP processing, process modelling, process and influence tables, AMFs etc. the handling of the uncertainties is discussed and decided upon. In the risk summation, most of the uncertainties are accounted for by studying variants and using cautious assumptions or by showing negligibility of the impact of the uncertainty.

As documented in table 13-3 of the SR-Site Main Report (SKB, 2011), only the following uncertainties[1] are directly propagated as probability distributions into the risk summation:

- Instantaneous release fraction
- Corrosion release fraction
- Corrosion release rate
- Fuel dissolution rate
- Concentration limits
- Rock diffusivities
- Rock partitioning coefficients
- Darcy flux at deposition hole
- Rock transport resistance
- Rock advective travel time

[1] The question of using or not using the EFPC rejection criterion is not addressed here; as pointed out by SKB this is not an uncertainty in the usual sense but rather a technological choice.

According to SKB's Radionuclide transport report (SKB, 2010b), 56 values for the

- Canister failure times

were each combined with 50 realisations of the transport calculations.
Apparently, the

- Number of failed canisters

(SKB, 2011), in (SKB, 2010b) named as "Average number of failed canisters" was directly used for calculating mean values from the releases obtained from the transport calculations.
All other input values were treated deterministically. Most of the distributions were directly taken from the data report, namely:

- Instantaneous release fraction
- Corrosion release fraction
- Corrosion release rate
- Fuel dissolution rate
- Concentration limits
- Rock diffusivities
- Rock partitioning coefficients

The hydrogeological data, namely

- Darcy flux at deposition hole
- Rock transport resistance
- Rock advective travel time

were directly derived from three hydrogeological models assuming different correlation structures between transmissivity and fracture size (uncorrelated, semicorrelated, correlated), for each of which several realisations were studied.
SKB argues: „Both the uncorrelated and the fully correlated models represent extremes of the correlation structure. In particular, the uncorrelated model lacks support in observations. The semi-correlated model used as the base case is seen as the most realistic representation, but it is not possible to quantify the degree of correlation in a rigorous manner. Therefore, the span represented by the three models is considered as a reasonable illustration of the conceptual uncertainties associated with the hydrogeological DFN models."
The two entities

- Number of failed canisters
- Failure times

were derived in a more sophisticated manner. These two uncertainties are strongly related to each other: The time of failure for each canister is the sum of the time needed for buffer erosion until advective conditions are reached and the time needed for corrosion until the canister is penetrated, and the canister counts as "failed" if its time of failure lies within the assessment timeframe.
Concerning <u>buffer erosion</u>, most uncertainties (dependency of erosion on groundwater cation charge concentration, time for which erosion occurs, amount of buffer necessary to reach advective conditions, dependency of erosion on flow and fracture aperture) were treated deterministically. In contrast, uncertainties / variability of the flow field were addressed using several realisations for each correlation structure (uncorrelated, semicorrelated, correlated) considered (SR Site Main Report, section 12.2.2). SKB then presents verbal statements and a figure (12-3) addressing average or mean numbers of emplacement positions with advective conditions, the mean values taken over the several realisations for the DFN models.
<u>Probability distributions for the corrosion rates</u> are presented in the SR-Site main report (SKB, 2011). Most of the findings in the following section were, however, drawn from the more detailed explanations in the Corrosion Calculations Report (SKB, 2010a).

4.3. The Consultants' assessment

Uncertainties concerning buffer erosion: The means and the bandwidths displayed in figure 12-3 (SKB, 2011) illustrate the epistemic uncertainty concerning the fracture distribution under certain model assumptions about the correlation structure, while the variation from case to case illustrates the epistemic uncertainty concerning the underlying correlation structure (plus other uncertainties mentioned above: time for which erosion occurs, amount of buffer necessary to reach advective conditions, fracture aperture). However, the entities transferred to the risk summation are not these mean values or bandwidths, but the erosion times calculated for each emplacement borehole for the several cases. The figure shows that the semicorrelated model yields more favourable results than the other two. Nevertheless, SKB uses this model (and not the other two) as starting point for the alternative cases. In the opinion of the reviewer, this is not consistent with SKB's otherwise cautious approach. (Remark: the caption of the vertical axis in the figure is confusing; the figure shows not only "mean numbers" but numbers in general).

In the opinion of the reviewer, the methodology for deriving probability distributions for the corrosion rates is a bit hard to understand when reading only the main report. From the more detailed explanations in the Corrosion Calculations Report (SKB, 2010a) the following can be concluded concerning the handling of uncertainties:

- Some corrosion mechanisms were excluded from further analyses on the basis of phenomenological arguments (e.g. about stress corrosion cracking) and / or scoping calculations enabling to bound the extent of corrosion (e.g. mass balance considerations). It is beyond the scope of this review to judge the adequacy of the underlying physico-chemical considerations. From an assessment methodology point of view the approach appears sound and in line with the "pessimistic estimate of uncertainty" as discussed in part 1 of the review.
- Several phenomenological uncertainties concerning the corrosion process have been addressed by using pessimistic or cautious assumptions (e.g. about reaction kinetics). Again, the reviewer is not in a position to judge about the underlying physico-chemical considerations but considers the methodological approach as sound and in line with the "pessimistic estimate of uncertainty" (see chapter 3).
- For the corrosion rates in the case of an intact buffer the following uncertainties have been explicitly accounted for:
    - Spatial variability of the flow field by presenting cumulative probability distributions (cumulative distribution functions, cdf) presented in figures 5-2 et al. (SKB, 2010a). Actually, these cdfs are expressions of the spatial variability (from emplacement borehole to emplacement borehole) of one single realisation (the so-called base case) for each of the various DFN models. Apparently, the authors interpret this spatial variability as probability distribution for each single canister (emplacement borehole) resulting from the variation of the flow field. In the view of the reviewer, this approach confuses spatial variability (of the very single base case flow field considered) with epistemic uncertainty (about the flow field itself). However, in geostatistics it is a common approach to assume stationarity of random functions (of position), i.e. invariance of certain characteristics of the random function under translations. Under such assumptions, statistics of one realisation derived by varying the position of interest (as for SKB's cdfs) can be used for characterising the

distribution of the random function. However, SKB does neither explain this approach and assumption nor justify a stationarity assumption. Such justification would have been possible by considering different realisations of the flow field (see below).

  - Epistemic uncertainty concerning the DFN model by presenting three different cdfs for DFN model variants (uncorrelated, semicorrelated, correlated) for the intact buffer but using the semicorrelated model as basis for the deterministic sensitivity cases (or variant considerations, see below). However, again the reviewer notes that the semicorrelated model yields the most favourable cdfs of the corrosion rates (intact buffer, figures 5-2 ff., SKB, 2010a) which implies that using this model does not fit with SKB's otherwise cautious approach.
  - (Epistemic) uncertainty concerning the fracture distribution by exploring realisations for each of the three DFN models mentioned above. Unfortunately, these results are not presented although they might serve as justification of the implicit stationarity assumption mentioned above.
  - Uncertainty concerning spalling by presenting two variants (spalling, no spalling) for each of the three cdfs mentioned above as well as by presenting an alternative pessimistic variant in which all the water in the spalling zone is equilibrated.
  - Uncertainty concerning the sulphide concentration by presenting a variant using the 90th percentile of the sulphide concentration distribution observed at Forsmark (as a kind of reference case) and another one using its maximum (described as very pessimistic since it postulates the presence of the maximum concentration at all positions).
  - Uncertainty concerning the transport resistance of the buffer by presenting a case for which no buffer resistance is assumed.

  For all these variants, the cdfs reach their maximum (=1) for corrosion rates considerably smaller than the rate necessary to penetrate the canister. Despite of the fact that obviously not all theoretically conceivable combinations of the variants described above were tested, the cdfs presented together with the very pessimistic (sometimes unrealistic) character of some of variants described above suggest the validity of the conclusion that the canisters will not be penetrated during the assessment period as long as the buffer remains intact. However, this conclusion could further be substantiated by also presenting results for DFN model realisations different from the base cases. In particular, this could just justify the above mentioned stationarity assumption underlying the cdfs presented for the corrosion rate.

- For the case of buffer erosion which, in contrast to the case with intact buffer, provides a non-zero contribution to the risk summation, the following uncertainties have been explicitly accounted for:
  - Spatial variability of the flow field by presenting cumulative probability distributions (cumulative distribution functions, cdf) presented in figure 5-6. (SKB, 2010a) (with two variants: use of the EFPC rejection criterion, and otherwise). In the perception of the reviewer, the cdf presented in figure 5-6 has, in contrast to the ones in figures 5-2 ff., a completely different role: While figures 5-2 ff. serve as argument for sufficient canister performance in case of an intact buffer, figure 5-6 serves only illustrative purposes. The cdf presented in the figure is not used for assessing

the risk contribution in the case of buffer erosion. While the reviewer's comments about spatial variability, epistemic uncertainty and stationarity apply as above, i.e. figure 5-2 addresses spatial variability rather than epistemic uncertainty, these findings are of no consequence with respect to the risk summation.

- Spatial variability of the flow field by presenting data for canister corrosion and buffer erosion times in tables 5-4 and 5-5(SKB, 2010a). The flow field has not only an impact on canister corrosion but also on the buffer erosion time (varying with emplacement position as discussed above). For the consequence calculations, the time of canister failure is defined by the sum of the erosion time and the corrosion time.
- Uncertainty concerning the sulphide concentration: According to SKB, these concentrations are uncorrelated with the fracture distribution: "No correlation was found between hydrogeological information on the fractures being sampled and the sulphide data." (SKB, 2010a) When addressing the combination of buffer erosion and corrosion times (tables 5-4 and 5-5, SKB 2010a), the sulphide concentrations are sampled for each borehole using their empirical distribution (based on measured data, see above). This was done for the base case as well as for one alternative realisation (table 5-5, see above). SKB then argues (SKB, 2010a):

  "In Table 5-4 the erosion and corrosion times are given for the 4 canister positions that could fail within 10^6 years, for the base case semi-correlated hydrogeological DFN model, and by applying the EFPC criterion. In Table 5-5 the corresponding erosion and corrosion times are given for the five canisters that fail within 10^6 years, for realisation r3 of semi-correlated hydrogeological DFN model, and by applying the EFPC criterion. It can be seen from the tables that the erosion and corrosion times are comparable for the highest sulphide concentration. For lower sulphide concentrations the corrosion times will increase, and thus largely determine the failure times."

  The interpretation of the reviewer is that SKB tested each sampled sulphide concentration for each borehole, by doing so deriving a probability distribution of the corrosion times separately for each single borehole. The tables then present the only combinations of flow rate (i.e. position) and sulphide concentration for which a failure occurs within the assessment timeframe. In the case of realisation r3 (table 5-5) eight such cases are presented but they concern only five boreholes (for four boreholes canister failure will only occur for the highest possible sulphide concentration, for one borehole for four different values of the sulphide concentration). The reviewer is of the opinion that this should have been explained more clearly in the documentation (e.g., the reader might misunderstand the method in a way that just one spatial distribution of the sulphide concentrations was sampled for, and combined with, each flow model realisation).
- (Epistemic) uncertainty concerning the DFN model and the fracture distribution by exploring variants for the semicorrelated DFN model (one presented in table 5-5 and discussed in an exemplified way (SKB, 2010a)) and by sensitivity studies concerning the choice of the correlation structure of the DFN

model and the choice of the realisation. For the sensitivity studies, mean numbers of failed canisters are presented for each calculation (all three correlation models, for each several realisations) in figure 5-7 (SKB, 2010a).
Again (as for the case of the intact buffer), one needs more clearly to distinguish between spatial variability of the flow field and epistemic uncertainty about fracture distributions. However, for the erosion case SKB presents not only the results for the semicorrelated base case DFN model but also for alternative models and several realisations, by doing so illustrating the impact of epistemic uncertainty. Rather systematically, the use of alternative (fully correlated and uncorrelated) models lead to results less favourable than for the semicorrelated model. Therefore, the reviewer wonders whether using the results of the semicorrelated model for the risk calculation fits to SKB's otherwise cautious approach.

- Uncertainties concerning the buffer loss required to reach advective conditions, duration of buffer erosion, fracture aperture, and initial advection by presenting comparisons for the mean number of failed canisters (and not the failure times, as indicated in the text) which show that the impact of these uncertainties is limited. The reviewer wonders whether combining two or more of such deviations would have led to different results.
- Uncertainty concerning the temporal evolution of the sulphide concentrations by "Assuming the mean value of *[HS−]* for all deposition positions, which is equivalent to assuming that *[HS−]* at a given position will vary over time with an average equal to the mean value of the entire *[HS−]*-distribution, i.e. $5 \cdot 10^{-6}$ M, yields no corrosion failures for the semi-correlated hydrogeological DFN model. Although it cannot be justified to assume a temporal variability that is represented by the given sulphide distribution, it is not unreasonable to assume that the sulphide concentrations would vary over time and thus serve to reduce the expected number of canister failures considerably." (SKB, 2010a) The reviewer is of the opinion that here, again, categories are confused: The mean values are derived from a spatial distribution but the argumentation refers to variation over time, thus assuming that the present spatial distribution is representative for the evolution over time to be expected. More precisely, the reviewer's interpretation of SKB's reasoning is as follows: The sulphide concentration will vary over time. Canister failure, however, only occurs for positions with relatively high concentrations assumed constant for the whole assessment time. If the spatial distribution is somehow representative for the evolution over time, this means that this evolution will lead to lower concentrations at these positions for considerable times, with the consequence that failure will most likely not occur even at these positions. The reviewer is of the opinion that the underlying assumption of representativeness is a little fragile. However, SKB uses this reasoning only for illustrative purposes and not for the risk summation; therefore this weakness is of little or no consequence.
- Uncertainty concerning the sulphide concentration distribution by modifying the distribution.

- o Uncertainty concerning the corrosion geometry by presenting a case with alternative (more pessimistic) assumptions.
- o Phenomenological uncertainty concerning corrosion at anoxic conditions by presenting what-if considerations concerning the corrosion depth.

Summary

In summary, about uncertainties concerning the flow field, the following can be stated: One needs to distinguish between (i) (epistemic) uncertainty about the fracture distribution and resulting flow field and (ii) its spatial variability of the fracture distribution (geometrical data and physical properties). For the former, there are two levels: (ia) the apparently unknown correlation between transmissivity and fracture size and (ib) the actual fracture distribution. The cdfs for canister corrosion rates presented account for (ii), (ia) is addressed by exploring three correlation models, and (ib) by exploring several DFN realisations for each of these models.

The cdfs (ii) play a major role when arguing that there is no risk contribution in the case of an intact buffer, (ia) is here accounted for since these cdfs are presented for each of the correlation models. An account for (ib) is however missing; only the so-called base cases (realisations) for each correlation model are presented. Therefore, the argumentation is to some extent based on a confusion of spatial variability with epistemic uncertainty and implicitly using a stationarity assumption which is neither discussed nor substantiated. A way of substantiating it could be to present the cdfs for the other realisations.

For the case of buffer erosion, which contributes to the risk summation, however, the cdfs do not play a role. Here, spatial variability (ii) is accounted for by studying the specific emplacement positions for which, dependent on the flow field, buffer erosion and canister corrosion can lead to a canister failure within the assessment timeframe. Uncertainty about the correlation structure (ia) is accounted for by sensitivity studies concerning the choice of the correlation structure of the DFN model, while the uncertainty about the fracture distribution (ib) is addressed by presenting results for various realisations.

The spatial distribution of the sulphide concentrations (iii) is addressed by "testing" all measured values for each emplacement borehole which leads to probabilistic statements. The temporal evolution of the sulphide concentrations is not explicitly addressed in the risk calculations, the concentrations are left constant. SKB argues that this is a cautious approach since only very high concentrations result in canister failure and it is likely that such high concentrations will not remain at the position in question over the entire timeframe. Although the reviewer considers it very likely that consequences were overestimated by applying this approach, a strict justification is lacking; it was not substantiated that the measured sulphide concentration values have indeed the same distribution as the sulphide concentrations expected in the future.

The risk contribution from the instant release fraction (IRF) is treated separately by calculating a mean dose based on the dose resulting from the IRF and an exposition probability based on the canister failure probability and accounting for the relatively short exposition duration. SKB then argues that the mean dose is "…more than four orders of magnitude below the dose corresponding to the risk limit. The pulse releases thus give negligible contributions to the probabilistically calculated mean dose." The reviewer is of the opinion that a comparison with the calculated mean dose for buffer erosion and corrosion rather than with the risk limit is of importance here. He is further of the opinion that the way deriving the exposure probability has by definition a potential for risk dilution, as acknowledged by SKB and addressed in section 13.9.4 of the SR-Site Main report (SKB, 2011).

SKB states further "The central output from the erosion/corrosion calculations is list of failure times and canister positions resulting from the combination of canister specific flowrates with the sampled sulphide concentrations. These results are transferred to radionuclide transport calculations … ." "Input distributions of failure times and geosphere transport data were obtained from the ten realisations of the semi-correlated DFN model, each yielding data for the ensemble of 6,000 canisters." (SKB, 2011). As shown in figure 13-21 (SKB, 2011) as well as in the ensuing viewgraphs showing calculated mean annual doses, the other two correlation models were explored as well. Given the fact that – as visible at various places – the use of the semicorrelated DFN model has a rather favourable impact on the erosion (see figure 12-3 in (SKB, 2011)) and corrosion (figures 5.2 ff. in (SKB, 2010a)) calculation results, the reviewer is of the opinion that it would have been advisable to address the cases with alternative transport model assumptions (Th mobility, colloids etc.) also for the other two correlation structures in order to better explore the space of uncertainties.

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APPENDIX 1

Coverage of SKB reports

Table 1: Coverage of reports

Reviewed report	Reviewed sections	Comments
SKB TR-11-01, Long-term safety for the final repository for spent nuclear fuel at Forsmark. Main report of the SR-Site project.	10.3.5, 10.3.6, 10.3.8, 10.3.12, 10.4.5, 10.4.6., 12.2.2, 12.3.2, 12.6.2, 13.2.4, 13.5.6	Systematic deterministic studies concerning the sensitivity of model assumptions, see introduction
	13.5.11	SA for the central corrosion case
	13.6.2	SA for canister failure due to shear load
	2.5.6, 2.8.1, 9	Approach for use of conservative and best-estimate parameter values
	3.	FEP processing with a view to uncertainty propagation
	5.-7., 12	Sources and role of phenomenological uncertainties and ways to propagate them into modelling
	12., 13	Propagation of uncertainties, addressing uncertainties concerning flow field, calculations concerning buffer erosion and canister corrosion, derivation of probability distributions and statements about failure times, propagation into risk summation
SKB TR-10-66, Corrosion calculations report for the safety assessment SR-Site.	1.2, 3, 4, 5	Phenomenological basis, methodology and results of corrosion calculations
SKB TR-10-66, Radionuclide transport report for the safety assessment SR-Site	4.4.2	Use of input data for probabilistic calculations
	4.4.3	Sensitivity analyses

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The Swedish Radiation Safety Authority has a comprehensive responsibility to ensure that society is safe from the effects of radiation. The Authority works to achieve radiation safety in a number of areas: nuclear power, medical care as well as commercial products and services. The Authority also works to achieve protection from natural radiation and to increase the level of radiation safety internationally.

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

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