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Technical Note

2012:36

Documentation and Traceability of Data in SKB's Safety Assessment SR-Site: Initial 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 i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Syftet med detta projekt är att granska SKB's dokumentation av data i säkerhetsanalysen SR-Site med utgångspunkt från den s.k. datarapporten. Relevanta aspekter av dokumentation av data innefattar exempelvis SKB:s metoder för att organisera och klassificera data i säkerhetsanalysen, referenshantering och spårbarhet från rapporter på lägre nivå och primära datakällor, kvalificering av indata samt kontroll av dataanvändning.

Författarnas sammanfattning

Den 16 Mars 2011 skickade Svensk Kärnbränslehantering AB in en ansökan om tillstånd för att uppföra och driva en inkapslingsanläggning för använt kärnbränsle i Oskarshamns kommun samt ett slutförvar för inkapslat använt kärnbränsle vid Forsmark i Östhammars kommun. SKB's ansökan granskas för närvarande vid Strålsäkerhetsmyndigheten (SSM) samt deras externa experter i det första steget av granskningen, den inledande granskningsfasen. Denna rapport innehåller en granskning av SKB's kvalitetssäkringskrav (QA) samt dokumentation och spårbarhet av data i säkerhetsanalysen SR-Site.

Denna gransking har utförts i tre steg. Först har kvalitetssäkringsplanen och styrande dokument för projektet granskats. Sedan har SR-Site:s datarapport granskats med fokus på dess målsättning, struktur och fullständighet. Till sist har stickprov av utvalda data genomförts med syftet att kontrollera spårbarhet av data i säkerhetsanalysen SR-Site.

Tolv kvalitetssäkringsrelaterade (QA) dokument har granskats i detta arbete. Rent generellt bidrar de undersökta dokumenten till en rimligt fullständig uppsättning krav avseende kvalitetspåverkande frågor kopplade till säkerhetsanalysen SR-Site, och om dess krav tillämpas på ett korrekt sätt inger detta förtroende för tillförlitligen hos säkerhetsanalysens resultat. Utvecklingen av kvalitetssäkringsrelaterade dokument och kvalitetskrav har dock pågått samtidigt som säkerhetsanalysen SR-Site har tagits fram, och detta har möjligen förhindrat en fullständig tillämpning av kvalitetsprocedurer samt har möjligen begränsat möjligheterna att genomföra fullständiga kvalitetsrevisioner av SR-Site projektet.

En viktig invändning är att kvalitetssäkringskraven för att tillhandahålla data till säkerhetsanalysen SR-Site har reviderats efter det att datarapporten hade publicerats. Datum för revisionen samt karaktären på de kommentarer i dokumentationen för revisionen antyder att införandet av data till datarapporten inte följde de uppsatta kraven och att kraven därför anpassats så att de motsvarade den procedur som faktiskt ägde rum. Syftet med SR-Site:s datarapport är att sammanställa, dokumentera, och kvalificera ingångsdata som identifierats som särskilt viktig för den långsiktiga säkerheten av ett KBS-3 förvar. Det finns dock ingen diskussion redovisad om de kriterier som de personer som arbetat med datarapporten har använt för att avgöra vilken typ av data som behöver sammanställas i datarapporten. Det finns inte heller dokumenterat vilka individer som har fattat beslut om att ta med data i datarapporten, och var sådana beslut har dokumenterats. Alla data som har identifierats som särskilt viktiga har dessutom inte presenterats i datarapporten, och det är nödvändigt att söka efter sådan information i en bredare uppsättning av SR-Site dokument. Det är ofta svårt att lokalisera sådan information eller att avgöra om sådana data har kvalificerats överhuvudtaget.

Spårbarheten hos ett urval av data i SR-Site:s datarapport har undersökts genom stickprov och granskning av underliggande referenser. Ett antal mindre fel och spårbarhetsfrågor har upptäckts, med det är osannolikt att dessa har så stor betydelse att de skulle påverka säkerhetsanalysens beräkningar eller argument som helhet. Det faktum att det finns flera mindre och undvikbara fel respektive spårbarhetsproblem skapar en oro för att det kan finnas oupptäckta mer betydelsefulla fel.

Sammanfattningsvis ifrågasätter granskarna värdet av datarapporten; en datarapport bör vara referens för alla data som används i säkerhetsanalysen och i denna bör alla parametrar diskuteras och kvantifieras fullt ut. I själva verket visar denna granskning att vissa data kvalificeras i datarapporten, och andra data kvalificeras i andra rapporter, medan data som SKB betraktar som mindre viktig för säkerhetsanalysen inte kvalificeras och sammanställs centralt överhuvudtaget. Rapporter inom säkerhetsanalysen citerar i vissa fall datarapporten och andra fall andra rapporter vilket innebär att datarapporten inte konsekvent används som den huvudsakliga källan.

Projektinformation

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Diarienummer ramavtal: SSM2011-4244
Diarienummer avrop: SSM2011-4548
Aktivitetsnummer: 3030007-4026

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 project is to review SKB's documentation of safety assessment data in SR-Site using the data report as a starting point. Relevant aspects of data documentation include for instance SKB's methods for organising and characterising safety assessment data, referencing and traceability from lower level reports and primary sources, qualification of input data as well as justification and control of data use.

Summary by the authors

On 16th March 2011 SKB applied for a licence to construct and operate a spent nuclear fuel encapsulation facility in Oskarshamn Municipality and a final repository for the encapsulated fuel at Forsmark in Östhammar Municipality. SKB's SR-Site safety assessment for the spent fuel repository is currently being reviewed by the Swedish Radiation Safety Authority, SSM, and its external experts in the first step of the review, the Initial Review Phase. This report provides a review of quality assurance (QA) requirements and data documentation and traceability in the SR-Site safety assessment.

The review has been carried out in three parts. First, the SR-Site QA plan and project steering documents were reviewed. Secondly, the SR-Site Data Report was reviewed, focusing on its stated objectives, structure and comprehensiveness. Finally, spot-checks of selected data sets were performed with the aim of checking data traceability in the SR Site safety assessment. Twelve QA documents were reviewed in this work. Overall, the reviewed QA instructions do provide reasonably comprehensive coverage of quality-affecting issues relating to the SR-Site safety assessment and, if implemented correctly, would generate confidence in the reliability of the safety assessment results. However, development of the QA documents and instructions has been ongoing during production of the safety assessment SR-Site, possibly hindering full application of the QA procedures and limiting opportunities for any comprehensive QA audits of the SR-Site project.

A key concern is that the QA instruction on supplying data to the SR-Site Data Report was revised after the Data Report was published. The revision date and the nature of the comments in the procedure revision history note indicate that the supply of data to the Data Report did not follow the requirements set out in the procedure and that the procedure was altered subsequently to match the process that did take place.

The SR-Site Data Report aims to compile, document and qualify input data identified as essential for the long-term safety of a KBS-3 repository. However, there is no discussion of the criteria that the SR-Site Data Report Team used to determine which data to include in the Data Report, or who made decisions on data inclusion and where such decisions are recorded. Further, not all data identified as essential are presented in the Data Report and it is necessary to locate information on such data in the broader suite of SR-Site documents. It is often difficult to locate such information or to determine if such data are qualified at all.

The traceability of selected data sets in the SR-Site Data Report was examined through spot-checks and examination of lower level supporting references. A number of minor errors and traceability issues have been identified in this selective review, although these are unlikely to be of such significance that they affect the calculations and arguments presented in the safety case. However, the number of such simple and avoidable errors and lack of traceability raises concerns that there could be significant undetected errors elsewhere.

Overall, the reviewers question the value of the Data Report; a safety assessment data report should be the reference document for all data used in the assessment and the parameters should be fully discussed and qualified. This review found some data are qualified in the Data Report, some data are qualified in other reports, and data regarded by SKB as unessential for the assessment are not qualified and centrally recorded at all. Further, some assessment reports cite the Data Report and some cite other SR-Site reports; the Data Report is not consistently the key source.

Project information

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Framework agreement number: SSM2011-4244
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Contents

1. Introduction

1.1. Background

On 16th March 2011 the Swedish Nuclear Fuel and Waste Management Company, SKB, applied for a licence to construct and operate a spent nuclear fuel encapsulation facility in Oskarshamn Municipality and a final repository for the encapsulated fuel at Forsmark in Östhammar Municipality. SKB's application is now being reviewed by the Swedish Radiation Safety Authority, SSM, and the Land and Environmental Court in Nacka. The Land and Environmental Court's review will be carried out on the basis of the Environmental Code. SSM is reviewing nuclear safety in the proposed facilities in accordance with the Nuclear Activities Act.

SSM intends to review SKB's safety assessment for the spent fuel repository, SR-Site, in a stepwise and iterative fashion. The first step is the Initial Review Phase where the overall goal is to achieve broad coverage of SR-Site and its supporting references and to identify the need for complementary information and clarifications from SKB. After the Initial Review Phase has been completed, SSM will determine if the quality and comprehensiveness of the safety assessment SR-Site is sufficient to warrant the planned in-depth assessment during the Main Review Phase. The Main Review Phase will consist of a number of review tasks defined to address uncertain and/or safety critical review issues that require a more comprehensive review treatment.

Due to the large scope and scientific breadth of the safety assessment, SSM has arranged for external experts to support them in their review. Staff at Galson Sciences Ltd (GSL) have previously supported SSM in its review of SKB's work to develop the repository concept (e.g., Baldwin and Hicks, 2009; 2010; Hicks, 2005; 2007; Hicks and Baldwin, 2008; Wilmot, 2003; 2011). GSL has been contracted to support SSM in its review of the SR-Site safety assessment, in particular with respect to documentation and traceability of data, handling of FEPs (features, events and processes), and corrosion of the copper canister disposal package. This technical report documents the Initial Phase review by GSL of data documentation and traceability in the SR-Site safety assessment.

1.2. Objective

The objective of this task is to review the sufficiency of SKB's documentation of data critical to the SR-Site safety assessment, as compiled in the Data Report (SKB, 2010a). The task also aims to examine the traceability of data in the safety assessment through spot-checks of selected data sets and examination of lower level references.

1.3. Approach and Report Structure

This review has been carried out in three parts. First, the SR-Site quality assurance (QA) plan and project steering documents were reviewed. The authors have previously reviewed SKB's QA plan and the QA procedures developed for use in the production of SR-Site (Baldwin and Hicks, 2009). The QA procedures reported in SR-Site were checked to see if any had been revised since the previous review and procedures that had been revised were reviewed again. The findings of this review are reported in Section 2.

Secondly, the SR-Site Data Report was reviewed, focusing on its stated objectives, structure and data selection (see Section 3). Finally, Section 4 presents the findings from spot-checks of selected data sets, considering data traceability in the SR-Site safety assessment, data transparency and appropriate use of data.

The key findings from this review of data traceability and transparency in SR-Site are summarised in the conclusion (Section 5). At the request of SSM, this report also includes three appendices. The first appendix records the SKB reports that have been reviewed in this work; the second appendix summarises the proposed requests for complementary information from SKB; and the third appendix lists proposed topics for further review in the Main Review Phase.

2. SR-Site Quality Assurance Documents

SKB has applied a management system that fulfils the requirements of ISO 9001:2000 (SKB, 2011a, §2.9) certified by DNV Certification AB, Sweden. Within this management system, SKB has applied a quality plan for the entire Spent Fuel Project (SKB document SDK-001) and, below this, has defined a quality assurance (QA) plan for the SR-Site project (SKB document SDK-003), which builds on the QA plan developed for the SR-Can project.

The authors have previously reviewed a draft QA plan for the SR-Site safety assessment, as reported in (Baldwin and Hicks, 2009), which included a series of steering and QA-related documents that were at various stages of development. Table 2.1 lists the QA documents that were reviewed during the course of that project.

The aim of the previous review was to consider whether the steering documents were sufficiently comprehensive that their application would ensure that the expected requirements of a QA programme would be met. For example, consideration was given as to whether appropriate application of these documents would ensure that transparency and traceability of information would be sufficient to enable judgments to be made regarding the reliability and validity of the safety assessment.

Table 2-2 in the SR-Site Main Report (SKB, 2011a) provides a list of steering and QA-related documents developed for the SR-Site project. In response to a request from SSM, on 23rd April 2012, SKB provided the latest versions of the QA documents that were previously reviewed as well as the following four additional documents listed in Table 2-2 of the Main Report (SKB, 2011a):

- #7 - List of experts (SKBdoc 1096716, Version 1.0, approved 08/02/2012).
- #8 - Review plan for SR-Site reports (SKBdoc 1182953, Version 1.0, approved 12/11/2008).
- #16 – Instruction for task descriptions for the safety assessment SR-Site (SKBdoc 11863027, Version 1.0, dated 18/12/2008).
- #17 - Final control of data used in SR-Site calculations/modelling (SKBdoc 1186612, Version 1.0, approved 6/04/2009).

Of the eight documents previously reviewed in 2008/09 and provided again by SKB in 2012, three are the same versions as previously reviewed and the remaining five have been revised. All of the SR-Site QA documents provided by SKB are listed in Table 2.1 and differences in version numbers compared to those previously reviewed are noted.

Table 2.1: SR-Site QA-related documents previously reviewed by Baldwin and Hicks (2009) and those reviewed in the present report (supplied by SKB on 23 April 2012).

#	SKBdoc	Title	Version Reviewed in 2008/09	Version Supplied in April 2012
1	1174832	SDK-001 Quality Plan for the Spent Fuel Project	Version 1.0, Approved, 30 June 2008	Same version
2	1064228	SDK-003 Quality Assurance Plan for the Safety Assessment SR-Site	Version 2.0, Approved, 03 July 2008	Version 3.0, Approved, 19 February 2009
3	1082126	Instruction for Development and Handling of the SKB FEP Database - Version SR-Site (Appendix 1 to SDK-003)	Version 1.0, Approved, 19 March 2008	Same version
4	1082127	Instruction for Developing Process Descriptions in SR-Site and SR-Can (Appendix 2 to SDK-003)	Version 1.0, Approved, 03 July 2008	Same version
5	1082128	Instruction for Model and Data Quality Assurance for the SR-Site Project (Appendix 3 to SDK-003)	Version 0.11, Preliminary Draft, 29 August 2007	Version 1.0, Approved, 23 April 2009
6	1082130	SR-Site Model Summary Report Instruction (Appendix 4 to SDK-003)	Version 0.4a, , Preliminary Draft, 29 August 2007	Version 2.0, Approved, 21 June 2011
7	1082129	Supplying Data for the SR-Site Data Report (Appendix 5 to SDK-003)	Two versions were reviewed: Version 0.8, Preliminary Draft, 18 October 2007, and Version 2.0, Approved, 20 October 2008	Version 4.0, Approved, 22 June 2011
8	1183027	Task Description for the Safety Assessment SR-Site (Appendix 6 to SDK-003)	Not previously reviewed	Version 1.0, Approved, 18 December 2008
9	1186612	Final Control of Data used in SR-Site Calculations/Modelling (Appendix 7 to SDK-003)	Not previously reviewed	Version 1.0, Approved, 6 April 2009
10	1186579	Qualification of "Old" References (Appendix 8 to SDK-003)	Version 0.1, Preliminary Draft, 19 November 2008	Version 1.0, Approved 03 December 2008
11	1182953	Review Plan for SR-Site Reports (Appendix 9 to SDK-003)	Not previously reviewed	Version 1.0, Approved, 12 November 2008
12	1096716	List of Experts	Not previously reviewed	Version 1.0, Approved, 08 February 2012

Each of the steering and QA-related documents provided are discussed in turn below.

During the previous 2008/09 review, comments on the SKB QA documents were given to SKB. SKB supplied responses prior to a QA meeting held at SKB's offices in Stockholm (held on 28 November 2008), which was attended by SKB and SSM staff and consultants. Where comments from the previous review are reproduced in the discussion below, relevant responses from SKB and discussions at the meeting are summarised.

2.1. SDK-001 Quality Plan for the Spent Fuel Project

The version of the quality plan supplied by SKB in April 2012 is the same as that reviewed in 2009 (Version 1.0, approved on 30 June 2008, document 1174832). Therefore, the same review comments hold as previously stated, with key comments repeated below.

1. The Spent Fuel Project is divided into sub-projects and operations within sub-projects may be conducted as activities according to activity plans (*Section 2.1.1*[1]). One such sub-project is 'Site-Project Oskarshamn' and the review queried whether investigations carried out at the Äspö Hard Rock Laboratory (HRL), the Bentonite Laboratory, and the Canister Laboratory are included in this sub-project, or whether they are separate sub-projects within the Spent Fuel Project. Further, the quality plan does not specify if the requirements on the realisation and analysis of raw data (*Section 2.1.2*), or controls on measuring devices (*Section 3.5*), apply to investigations at the HRL, the Bentonite Laboratory, the Canister Laboratory and other laboratories involved in experiments in support of the repository development programme.

   In response (November 2008), SKB stated that the HRL, the Bentonite Laboratory and the Canister Laboratory are not part of the Spent Fuel Project but that they do follow the SKB quality management system and there are specific procedures for their activities. SKB's data handling procedure requires that, before a data set is given QA clearance for use in the SR-Site safety assessment, checks are made on the data controls carried out by a contractor when data are delivered and a further check is made when data are entered into the SICADA database. Depending on the nature of the data, tools linked to the database can be used to review the data.

2. The discussion of document review procedures (Section 4.4) indicates the types of review required for safety analysis reports. However, it is not clear if there are specific review procedures and criteria for SKB's TR-, R-, P- and IPR-series reports in addition to those for safety analysis reports. In particular, it is not clear if there are review requirements for reports that support, but are not part of, a licence application. For example, the review requirements for reports that document the application of models for detailed assessments of particular processes or which may involve the abstraction of parameter values for the safety assessment are not discussed. In addition, the QA plan does not mention if there is a process for addressing review comments.

   In response, SKB stated that reviews and/or referrals are made on all SKB reports. SKB explained that reports that are included in the licence application,

[1] References to sections within the SKB QA documents under review are presented in italics.

and supporting references within those documents, are reviewed according to special procedures in the quality management system. The review process includes a factual review, a quality review and an integrated review with other documents. For documents included in the preliminary safety report, a primary safety review and an independent safety review are made according to regulations (SKIFS 2004:1) concerning safety in nuclear facilities.

Subsequent to the above response from SKB, the revised SR-Site QA Plan (discussed in the next sub-section) states that all reports produced in the SR-Site project are subject to peer review, and a review plan for SR-Site has now been established as Appendix 9 to the QA plan (see Section 2.11).

3. The QA plan includes a discussion of non-conformities (Section 9). Documents that describe how non-conformities are to be managed and resolved are noted but there is no discussion of how non-conformities are identified within SKB. Also, it is not clear if audits are undertaken to identify non-conformities.

   SKB noted that data errors discovered, for example, during modelling work, are reported and addressed. Also, non-conformities can be identified and reported by all SKB staff and non-conformities relating to contractors' work are reported to SKB if they are relevant to the task. Internal audits and third-party audits are made according to the SKB audit plan, which is approved annually by the president of SKB.

   Again, subsequent to this response, the revised SR-Site QA plan now includes a section on QA audits (discussed below).

2.2. SDK-003 Quality Assurance Plan for the Safety Assessment SR-Site

Version 3.0, dated 19 July 2009, was supplied by SKB in April 2012, which is a more recent version than that previously reviewed (Version 2.0, approved on 03 July 2008).

The review of Version 2.0 had two main comments. The first considered that it was not clear how often project QA audits are carried out and there was no discussion of previous audits (e.g., the number of audits carried out to date and identification of, and response to, any significant non-conformities). A new *Section 2.3*, QA Audits, in Version 3.0 of this procedure states that internal QA audits are conducted according to a programme approved by the managing director of SKB, although this does not give an indication of audit frequency. *Section 2.3.1* provides a history of QA audits performed, which states that an audit took place in September/October 2008 and identified four non-conformities (this audit was noted by Baldwin and Hicks, 2009). The QA document also states that a second internal QA audit was ordered by the SR-Site project to be held during the first half of 2009; this document is dated July 2009 but there is no indication if the second audit took place.

Secondly, the discussion on peer review in Version 2.0 stated that several reports will be subject to peer review in SR-Site, but the criterion for deciding whether or not a report should be subject to such a review was not explained. The revised procedure (Version 3.0) states that all reports produced in the SR-Site project are subject to peer review within the project prior to being finalised. A review plan has also been established as Appendix 9 to the QA plan and is discussed below (see Section 2.11). The review plan defines the document that should be provided to the reviewers, general criteria for acceptance of a report, requirements on reviewers' competence and how the review documents shall be handled.

2.3. Instruction for Development and Handling of the SKB FEP Database – Version SR-Site

The version of this instruction supplied by SKB in April 2012 is the same version as that reviewed in 2009 (Version 1.0, approved on 19 March 2008, document 1082126, Appendix 1 to the QA Plan). Therefore, the same review comments hold as previously stated and the main comment is repeated below.

The development of the SKB FEP database for SR-Site focuses on the NEA FEP database. The review questioned why FEP databases that are not included in the NEA database, such as the database developed in support of the recent Yucca Mountain repository licence application, have not been considered.

SKB responded that it was felt necessary to freeze the input to the FEP work and considered that more recent FEP databases do not provide significant new input. SKB believes that this is also the case for the database developed in support of the Yucca Mountain repository licence application, because the conditions for this repository differ from those relevant to a Swedish repository (although SKB did note that earlier versions of the Yucca Mountain FEP database are included in the NEA FEP database).

2.4. Instruction for Developing Process Descriptions in SR-Site and SR-Can

The version of this instruction supplied by SKB in April 2012 is the same version as that reviewed in 2009 (Version 1.0, approved on 03 July 2008, document 1082127, Appendix 2 to the QA Plan). Therefore, the same review comments hold as previously, with key comments repeated below.

1. The instruction states that FEPs and matrix interactions can be screened out if they are 'of small importance for the evolution of the system', and that a 'motivation for such a judgment must be given' (Section 4.3). Other sections of this instruction outline the handling of documentation for each FEP. However, the procedures and criteria to determine whether a FEP (or matrix interaction) can be screened out of the safety assessment calculations are not specified. For example, it is not clear if there are requirements for clear and traceable documented quantitative or qualitative arguments for concluding that a particular FEP or interaction is of little consequence to the dose calculations, or is unlikely to occur. Also, it is not clear if guidance is provided to the experts on what is considered to be of low consequence to the dose calculations or low probability of occurrence.

   In response, SKB noted that the FEP handling procedure is described in *Sections 3.5* and *5.1* of the instruction and that there are requirements on documentation of the arguments in the FEP database. According to SKB, a judgment is made regarding whether the FEP or matrix interaction is important for the process in question. If so, it should be addressed in, or covered by, the process description where arguments for further handling of the process are given. No guidance is given to the experts on what is considered to be low consequence to the dose calculations, because SKB believes that judgments are primarily concerned with importance for the process and importance for the evolution of the system, but not the consequence to dose calculations.

2. The discussion of the structure and content of process descriptions (*Section 4.4*) does not mention if there is any requirement to ensure that the handling of processes and uncertainties in the safety assessment is consistent with the discussion and parameter values presented in the Data Report. If not, it may be possible that different experiments and parameter abstractions are used in the Process and Data Reports to derive different distributions for the same parameter.

   SKB indicated that the role of the process description is to describe the process and how the process will be handled (supported by appropriate arguments), and to describe the types of uncertainties associated with the suggested handling of the process. However, no parameter extractions or quantifications of data or uncertainties should be made in the process descriptions; SKB stated that the Data Report will quantify data and uncertainties whilst the Model Summary Report will provide the parameters for which quantitative data are required.

2.5. Instruction for Model and Data Quality Assurance for the SR-Site Project

Version 1.0, dated 23 April 2009, was supplied by SKB in April 2012, which is a more recent version than that previously reviewed (Version 0.11, a preliminary draft produced on 29 August 2007, document 1082128, Appendix 3 to the QA Plan). Note there has been a slight change in the title, from "Instruction for Model and Data Quality Assurance for the SR-Site Project" in Version 0.11 to "Plan for Model and Data Quality Assurance for the SR-Site Project" in Version 1.0.

1. SKB states in *Section 1* that computational tasks are identified in the Assessment Model Flowcharts (AMFs), which illustrate how key tasks are related and how data are used. However, other kinds of calculations are also performed; for instance, conversion of units, pre- and post-processing of data or other kinds of simpler, easily verified calculations. SKB states that these simpler calculations, although necessary for the assessment, are not regarded as assessment calculations and hence are not covered by this QA routine. It is unclear if these calculations are subject to any other QA procedure.

2. SKB maintains a centralised model storage area where models, source codes and other kinds of files, such as Excel spreadsheets, are stored (*Section 1*). However, SKB does not require codes used and owned by contractors to be stored in the model storage area. In this case, it is unclear how SKB ensures that it has access to the models used in the assessments and that it is not dependent on a single contractor for models. Further, it is not clear if SKB independently audits the models used by contractors.

3. An issue tracking system is used mainly for code development but also in combination with data storage where errors in codes and data are reported. However, it is stated (*Section 1*) that there exists no separate QA instruction for the issue tracking system and that use of the issue tracking system is not mandatory. Thus, it is unclear how else SKB tracks errors in data and codes if the issue tracking system is not used. It is also unclear who is responsible for

maintaining the issue tracking system and updating it if a member of SKB staff or a contractor notifies SKB of an error, or how interested parties are notified of the issue.

4. In the discussion on AMFs (*Section 4*), SKB notes that due to the nature of the safety assessment project, the AMFs will be continuously updated and that the teams behind the Model Summary Report and the Data Report are responsible for updating the AMFs. As stated in *Section 1*, the AMFs are used to identify the data that are to be included in the Data Report. However, it is not indicated how AMF updates are communicated between the two teams and more widely amongst those involved in developing the SR-Site safety assessment.

5. In review of Version 0.11 it was noted that the discussion of analysis documentation (*Section 10*) clearly defined the key information that should be recorded in the calculation reports, but did not specify if there are requirements for review and checking of the analysis documents.

   In response, SKB noted that the analysis documentation is used to record the results of computational tasks and that a template for the analysis documentation is provided. However, SKB also noted that it is not compulsory to produce a separate analysis document because this information should normally be included in the report in which the calculations are described. As such, the documentation will be reviewed in connection with the review of the report.

   Nonetheless, the authors consider that checking and review requirements should be specified for the situation where an analysis document is produced in addition to the calculation report and it contains information not provided in the calculation report. Such requirements are not specified in the revised Version 1.0 instruction.

2.6. SR-Site Model Summary Report Instruction

Version 2.0, dated 21 June 2011, was supplied by SKB in April 2012, which is a more recent version than that previously reviewed (Version 0.4a, a preliminary draft produced on 29 August 2007, document 1082130, Appendix 4 to the QA Plan).

The review of Version 0.4a had one main comment, which concerns the same point discussed in the preceding sub-section. The discussion on the assessment model flow charts (*Section 2.1*) states that minor calculation tasks performed in the assessment, such as post-processing of results, are not regarded as critical for the quality of the assessment and so are not included in the Model Summary Report. However, no mention is made of any requirements for checking these minor calculations or any checks that are carried out as part of the document checking and review process.

Previously, SKB responded that minor calculations are excluded from the Model Summary Report for practical reasons. The Model Summary Report defines such calculations as "…could be verified by simple hand calculations…" and the extent to which they are checked in the review process is controlled by the review criteria for the document in question. However, document review criteria are defined on an individual report basis and so minimum review requirements for checking of minor calculations should be stated in the QA instruction.

Also, two comments are made with regard to the version history of this instruction.

- The register of revisions (*Section 5*) in the Instruction records Version 1.0 as being produced on 29 August 2007, which is the same date as was stated for Version 0.4a reviewed in 2008/09.
- The latest version of the Model Summary Report Instruction, Version 2.0, is dated 21 June 2011 yet the SR-Site Model Summary Report (SKB, 2010b) was published in December 2010 and the Main SR-Site Report (SKB, 2011a) in March 2011. The comments on the revision history note that minor updates have been made based on experience from SR-Site; it is unclear why such experience is used to update a document that should be a relatively static procedural reference during the course of the project. Experience gained should not be used to revise the QA instruction after the process is complete, but should be recorded elsewhere; the procedure should only be revised if during the course of the project it is discovered that the procedure needs improvement for use in SR-Site.

2.7. Supplying Data for the SR-Site Data Report

Two versions of this QA document were reviewed in 2008/09. Initial comments were made on a preliminary version (Version 0.8, produced on 18 October 2007, document 1082129). Subsequent review comments were made on an approved version (Version 2.0, dated 20 October 2008). Version 4.0, approved on 22 June 2011, was supplied in April 2012. This instruction forms Appendix 5 to the QA Plan (SDK-003).

1. Review of the revised QA document found that the text has been extensively revised and clarified, with increased use of diagrams and examples. However, a few queries have been identified.

2. The previous review of this QA instruction noted that the flow of information between the Data Report and the data-supplying reports was unclear, and in particular it is unclear if there are any procedures for revising these reports and for ensuring that parameter values and distributions are used consistently throughout the safety assessment. However, the process to be followed is now more clearly defined in Version 4.0.

3. A statement is made in *Section 2* that the "Data Report does not concern all data used in the SR-Site safety assessment, but [only] those which are identified to be of particular significance for assessing repository safety". However, whilst it is stated that data are identified through analysis of the AMFs and the radionuclide transport assessment, there is no discussion of the criteria that are used to determine which data are to be included in the Data Report or who will make the decision on which data to include (i.e. the Data Report Team, the data supplier, or both).

4. Regarding experience from SR-Can, SKB notes that for SR-Site it is sufficient to state the conditions for which data were used in SR-Can modelling without justification as to why those conditions were studied (*Section 2.2.1*). However, understanding the conditions for which data are used is integral to the quality assurance of the data and, if not explained in the Data Report, detailed references should be supplied to the location of such a discussion.

5. *Section 2.4.1* of the QA document discusses qualification of supporting data. A 'value' is ascribed to supporting data that reflects the reliability of the data. However, it is unclear how the 'value' of the data is defined. From the instruction it is not clear if value judgments are qualitative or if there are procedures for assigning a value to data acceptability, although subsequent review of Data Report parameters (see Section 4) suggests that supporting data are categorised as such based on the judgment of the data supplier. Also, it is not clear if there is a value at which data are considered unacceptable.

6. The revised discussion in *Section 2.4.1* states that data taken from "widespread textbooks, which are considered to be established facts, need not to be scrutinised". While such data may be widespread in use, appropriate references should still be supplied.

7. In the revised QA document it is indicated that, when giving instructions to the supplier representative (who supplies qualified data to the Data Report), issues concerning natural variability of data or bias issues associated with data interpretation should be discussed at the discretion of the supplier representative (*Sections 2.7* and *2.8*). Such a decision should properly be discussed with the customer representative (the SR-Site team responsible for performing the safety assessment) and/or the Data Report Team (a subgroup to the SR-Site team) in order to determine the significance of the data set variability/bias.

8. SKB notes in *Section 2.1.1* that "as a result of the extensive work that will be conducted up to near completion of the SR-Site safety assessment, details of the models and model chain may be modified. As a result, this text [SR-Site modelling activities in which the data will be used] may have to be finalised in a late stage of the Data Report project. Thus only a preliminary version is provided early on to the supplier". It is unclear whether, once the text specifying the intended use of the data is finalised, the supplied data is checked against the revised specification for any incompatibility.

9. The latest version of this instruction, Version 4.0, is dated 5 May 2011 yet the SR-Site Data Report (SKB, 2010a) was published in December 2010 and the Main SR-Site Report (SKB, 2011a) in March 2011. The comments in the procedure revision history note that the responsibility for data qualification approval has been redefined and that a number of demands on the supplier and/or customer have been softened to reflect Section 2.3 in the Data Report (SKB, 2010a). This implies that the supply of data to the Data Report did not follow the requirements set out in the procedure and that the procedure was altered subsequently to reflect the process that did take place; it is unclear why this was done. The QA instruction for the supply of data to the SR-Site Data Report should be a relatively static procedural reference, possibly subject to revision during the course of the project, but should not require revision following completion of the activity for which it was written. It is not clear which parameters were produced to the original, more stringent, procedure and for which parameters the revised procedure was required.

10. A number of cells in the register of revisions table state “see head of first page”. Whilst this may be a valid statement for the current version of the document, it is not helpful for historical traceability. In this instance the production date for Version 3.0 of the instruction is unknown and it is therefore unclear if it was Version 2.0 or 3.0 that was the reference for the majority of the Data Report development period.

2.8. Task Descriptions for the Safety Assessment SR-Site

Version 1.0, approved on 18 December 2008, was supplied in April 2012 (document 11863027). This QA instruction has not been previously reviewed. This instruction forms Appendix 6 to the QA Plan (SDK-003).

This document sets out a logical structure for the customer and supplier to jointly define computational tasks, inputs and deliverables.

2.9. Final Control of Data Used in SR-Site Calculations/Modelling

Version 1.0, approved on 6 April 2009, was supplied in April 2012 (document 1186612). This QA instruction has not been previously reviewed. This instruction forms Appendix 7 to the QA Plan (SDK-003).

An instruction to return and verify that preliminary data used in assessments has been updated to be consistent with the final data presented in the Data Report builds confidence in the safety assessment.

SKB states in *Section 3* that the person in the SR-Site team in charge of the analyses/calculations to be controlled is also responsible for assigning someone to do the final control of the data and for storing the documentation of the data control. It is unclear how it is determined which analyses/calculations are subject to control and how it is ensured that all data sets based on preliminary data are checked. A central list of the data used in assessments and the data set version supplied would support this procedure. Further, the process to be followed if the calculations are complete but the preliminary data used are different from the final data should be defined.

2.10. Qualification of “Old” References

Version 0.1, a preliminary draft produced on 19 November 2008 (document 1186579) was reviewed in 2008/09. This document was reviewed at a later date than the preceding documents and, in the time available, it was not possible for SKB to provide a response to these comments. Version 1.0, approved on 3 December 2008, was supplied in April 2012. This instruction forms Appendix 8 to the QA Plan (SDK-003).

The instruction on qualification of old or external documents for use in SR-Site is necessary to ensure that the work performed prior to the introduction of the data quality assurance system, or by organisations external to SKB, is demonstrably fitfor-purpose. The instruction recognises that "old documents or parts of old documents can be made quality approved by conducting a documented factual review of the document or parts of the document that are referenced" (*Section 1*), but it is subsequently stated that this is judged "not possible…considering the substantial amount of time and resources it would require". The proposed alternative procedure, which involves qualification of references in the report where the references are used and review of that qualification by the experts selected for factual review of the report in question, appears sufficient. However, the difference in the resources required for each approach is unclear and there is potential for the proposed approach to lead to the qualification process being applied to a supporting reference more than once if the reference is cited in different SR-Site reports.

2.11. Review Plan for SR-Site Reports

Version 1.0, approved on 12 November 2008, was supplied in April 2012 (document 1182953). This QA instruction has not been previously reviewed. This instruction forms Appendix 9 to the QA Plan (SDK-003).

The instruction states that report reviewers are selected by the member of the SR-Site team responsible for the report and must have sufficient competence within the area covered by the report to judge whether the defined acceptance criteria are filled. However, there is no statement as to whether the selected reviewer must be independent of the work performed, outside of the SR-Site team or external to SKB.

2.12. List of Experts

Version 1.0, approved on 8 February 2012, was supplied in April 2012 (document 1096716). This QA instruction has not been previously reviewed.

This QA document contains lists of the experts contributing to the safety assessment SR-Site, either as members of the project team, as authors of reports produced within the project or as reviewers of such reports. Supporting traceability, the tables also contain clear reference to the documentation used to select the experts (e.g. a *curriculum vitae* of relevant professional achievements).

2.13. Summary

Overall, the reviewed set of QA documents and instructions do provide reasonably comprehensive coverage of quality-affecting issues relating to the SR-Site safety assessment and, if implemented correctly, would generate confidence in the reliability of the safety assessment results. However, development of the QA documents and instructions has been ongoing during production of the safety assessment SR-Site, possibly hindering full application of the QA procedures and opportunities for any comprehensive QA audits of the SR-Site project.

A number of review comments have been made during this review but the key points summarised below generally exclude comments that relate to procedures applied during development of the safety assessment (since SR-Site is now complete) and concentrate on those where further clarification is sought.

- The revised SR-Site QA plan (Section 2.2) includes discussion of QA audits, but does not give an indication of audit frequency. The document also states that an internal QA audit was ordered by the SR-Site project to be held during the first half of 2009, but there is no indication that the audit took place, despite the QA plan dating from July 2009. It should be clarified with SKB if the audit took place, what the findings were and if there were any non-conformities to be addressed.

- It is unclear if those calculations not subject to the Instruction for Model and Data QA (Section 2.5), e.g., pre- and post-processing of data or other kinds of simpler, easily verified calculations, are subject to any specific QA procedure, particularly if such calculations are not documented in the assessment reports. It should be verified that these calculations have been independently checked.
- SKB does not require codes used and owned by contractors to be stored in the centralised model storage system. It should be clarified how SKB ensures that it has access to the models used in the assessments and that it is not overly dependent on a single contractor for models. Further, it is unclear if SKB independently audits the models used by contractors.
- The SR-Site Data Report only includes data identified by SKB to be of particular significance for assessing repository safety. However, there is no discussion of the criteria that are used to determine which data are to be included in the Data Report or who will make the decision on which data to include (i.e. the Data Report Team, the data supplier, or both). This hinders data traceability in the assessment (see Section 3 for further discussion of this issue).
- The Data Report QA instruction states issues concerning natural variability of data or bias issues associated with data interpretation should be discussed at the discretion of the supplier representative. Such a decision should properly be discussed with the customer representative (the SR-Site team responsible for performing the safety assessment) and/or the Data Report Team (a subgroup to the SR-Site team) in order to determine the significance of the data set variability/bias.
- A key concern in this review is that the QA instruction on supplying data to the SR-Site Data Report was revised after the report was published (Version 4.0 is dated May 2011 yet the SR-Site Data Report was published in December 2010). The comments in the procedure revision history note that the responsibility for data qualification approval has been redefined and that a number of demands on the supplier and/or customer have been softened to reflect the Data Report content. This implies that the supply of data to the Data Report did not follow the requirements set out in the procedure and that the procedure was altered subsequently to reflect what did take place. The QA instruction for the supply of data to the SR-Site Data Report should be a relatively static procedural reference, possibly subject to revision during the course of the project, but should not require revision following completion of the activity for which it was written. It is not clear which parameters were produced to the original, more stringent, procedure and for which parameters the revised procedure was required. This requires clarification from SKB.

3. SR-Site Data Report

The SR-Site Data Report (SKB, 2010a) aims to compile, document and qualify input data identified as essential for the long-term safety of a KBS-3 repository. SKB (2010a, §1.1) aims to provide the data for a selection of relevant conditions and to qualify the data in a traceable fashion using the standardised procedures discussed in Section 2.

SKB (2010a, §1.3) states "trivial data" are not handled in the Data Report whilst, as mentioned previously, a statement is made in the QA instruction "Supplying Data for the SR-Site Data Report" that the "Data Report does not concern all data used in the SR-Site safety assessment, but [only] those which are identified to be of particular significance for assessing repository safety".

In agreement with the SR-Site Main Report, the Data Report (SKB, 2010a, §1.1.1) states that the data to be used in the quantification of repository evolution and in dose calculations are selected using a structured procedure. The process followed by SKB to identify essential data is described in Section 1.2.2 of the Data Report and was performed in two ways. The primary approach consisted of analysing the two assessment model flowcharts (AMFs; SKB, 2010a, Figures 2-1 and 2-2). SKB (2010a, §1.2.2) acknowledges limitations in this approach resulting in peripheral data that may be of importance for the safety assessment not being included in the Data Report, but reported elsewhere (e.g., the biosphere data constituting the background for estimating the landscape dose conversion factors are not reported; a decision was taken by SKB to limit the scope of the Data Report to include the estimated landscape dose conversion factors as the only biosphere-related data).

Secondly, a parallel approach was used for identifying input data to radionuclide transport modelling – all input parameters of the computational codes COMP23 and FARF31 were examined. SKB (2010a, §1.2.2) states that many of the associated data are qualified in the Data Report, while some inputs are taken from other sources. This parallel approach in a systematic way is new in SR-Site and SKB states (2010a, §1.2.2) that this was implemented to address regulatory review comments on the SR-Can Data Report: "a more complete version is needed prior to SR-Site, where the extent and limitation of the presentation is clearly justified".

The presentation in the SR-Site Data Report is improved but there is no discussion of the criteria that the SR-Site Data Report Team used to determine which data to include in the Data Report, or who made the decision and where it is recorded. There does not appear to be a central list of all the data reviewed by the SR-Site Data Report Team to determine if the data were sufficiently significant to include in the Data Report or not.

SKB (2010a, §1.2.2) states that the parallel approach to identifying essential data has resulted in an extended data inventory compared to the SR-Can Data Report. SKB also states that, based on SR-Can experience, a few data sets have been excluded from the report. However, these inventory differences are not specified. From a brief comparison of the table of contents in both reports (SKB, 2006a; 2010a):

- The Spent Fuel chapter now includes a section on corrosion release fraction data.
- The Canister chapter now appears to exclude sections on copper physical data, cast iron physical and mechanical data, and corrosion parameters.

- The Buffer and Backfill chapter now excludes sections on the thermal properties of the buffer and the mechanical properties of buffer and backfill.
- The content of the Geosphere chapter appears to be generally the same, although is approximately twice the size.
- A new chapter on Surface System Data has now been included.

As not all data identified as essential are qualified and presented in the Data Report, in some cases it is difficult to find where in the suite of SR-Site documents specific data are presented, or even if the data are qualified at all. Section 2.1 (SKB, 2010a) notes that a large quantity of spent fuel data are qualified in the Spent Fuel Report (SKB, 2010c); the majority of the data concerning the canister are qualified in the Canister Production Report (SKB, 2010d); and other backfill and buffer data (e.g., geometries and compositions) are qualified in the Buffer Production Report (SKB, 2010e) and the Backfill Production Report (SKB, 2010f). However, without a reference table recording the report in which each parameter is qualified (or is not regarded as essential and is therefore not qualified at all), it is necessary to search a number of reports to find the data qualification for a specific parameter. In addition, reports other than the Data Report do not always have clearly marked sections discussing qualification of individual parameters.

In review of the SR-Can Data Report, the regulators found it difficult to separate expert judgment made by the SR-Can Team in the Data Report from that made by the experts authoring the supporting documents (SKB, 2010a, §1.3). For this reason, SKB has modified the structure of the SR-Site Data Report to, as far as possible, separate the views of experts supplying the data from the views of the SR-Site Team. Each data set in the report is presented using a standard structure:

1. Modelling in SR-Site
2. Experience from SR-Can
3. Supplier input on use of data in SR-Site and SR-Can
4. Sources of information and documentation of data qualification
5. Conditions for which data are supplied
6. Conceptual uncertainty
7. Data uncertainty due to precision, bias and representativity
8. Spatial and temporal variability of data
9. Correlations
10. Result of supplier's data qualification
11. Judgements by the SR-Site team
12. Data recommended for use in SR-Site modelling

The above structure is discussed in Section 2.3 of the Data Report (SKB, 2010a) and in the relevant QA instruction reviewed in Section 2.7 of this report. The "source of information" section that was found to be useful in review of the SR-Can Data Report (Hicks and Baldwin, 2008, §3) has now been implemented for all data sets. The data qualification process defined appears logical and allocates responsibilities clearly, with good use of the supplier, customer and SR-Site Team terminology. A data qualification meeting held to formally decide and record delivery of data to SR-Site improves clarity and traceability. However, it is not clear what review criteria or procedures were used by attendees at the data qualification meeting to determine whether a particular data set is acceptable. It would also aid transparency if the SKBdoc number for the internal record of each data qualification meeting was recorded in the Data Report discussion for each parameter, which is not currently the case.

A footnote in the Data Report (SKB, 2010a, p.36) acknowledges, without explanation, that during production of the report the QA instruction for supplying data to the Data Report was updated to reflect the actual data qualification process applied. However, as discussed in Section 2.7 of this report, revising the QA instruction for data qualification to reflect what was done, rather than following the defined procedure, is not the way in which a QA system should be implemented. This change should be explained and justified. Further, it is not clear which parameters were produced under the original procedure and which to the revised procedure; the lack of a revision history section in the Data Report hampers traceability of this issue.

In addition, it should be clarified whether data not included in the Data Report, whether regarded as essential or not, are subject to any QA requirements (other than general review of the report in which it is presented). As defined in the SR-Site QA documentation (see Section 2), only data regarded as essential and presented in the Data Report appear to be covered by specific data QA requirements.

The key conclusion of this review for the Data Report as a whole is that the Data Report appears to not be quite one thing or another – it is expected that a safety assessment data report would be the reference document for all data used in the assessment, but that is not the case, and not all the parameters presented are fully qualified in the Data Report. Some data are qualified in the Data Report, some data are qualified in other reports, and data regarded as unessential for the assessment are not qualified and centrally recorded at all. Further, some assessment reports cite the Data Report and some cite other SR-Site reports; the Data Report is not consistently the key source. From the report title, it would be expected that the Data Report would provide the primary source of data for the assessment and that other reports in SR-Site would refer to relevant sections of the Data Report when analysing specific processes and scenarios. There has been modest improvement in this direction for some parameters (discussed in the next section) but, as found for the SR-Can Data Report (Hicks and Baldwin, 2008, §5), many of the SR-Site initial state and process reports contain comprehensive data discussions and do not always make use of data presented in the Data Report. Further, it appears that a number of data sets have been included in the Data Report after the related assessment has been completed – the Data Report was not the reference data source for the assessment. In fact, many of the SR-Site modelling reports have the same, or earlier, publication date as the Data Report (December 2010). Considering the way in which the SR-Site Data Report has been developed and applied, as compared with expectations for a safety assessment database, the reviewers question the usefulness of the Data Report for the producers of the safety assessment.

4. Traceability of Selected Data Sets

The traceability of selected data sets in the SR-Site Data Report was further examined through spot-checks and examination of lower level references. The choice of which data sets to examine in this review was arbitrary and limited by the time available for the Initial Review Phase, although some data sets were selected by drawing on the experience gained from previous reviews of parameters in the SR-Can Data Report (Hicks and Baldwin, 2008) and by considering parameters key to SR-Site.

The following sub-sections examine the traceability and reliability of data on spent fuel (SKB, 2010a, §3), the canister (SKB, 2010a, §4), the buffer and backfill (SKB, 2010a, §5), and the geosphere (SKB, 2010a, §6).

4.1. Spent Fuel Data

4.1.1. Selected Inventory

The Data Report (SKB, 2010a, §3.1.4) states that the data presented are qualified in the Spent Fuel Report (SKB, 2010c) and that scrutiny of lower level references is part of the qualification process of that report. However, there is no discussion in the Spent Fuel Report of the qualified or supporting nature of the references drawn upon, or the nature of any review or checks undertaken. Indeed, the Spent Fuel Report relies heavily upon data supplied directly from the Swedish nuclear power plant operators and unpublished SKB documents. It is acknowledged that at least one of these documents is unpublished due to the sensitive nature of its contents (SKBdoc 1219727 v2.0), but the private communication and unpublished nature of these information sources results in a lack of transparency and traceability in the data presented and hinders review.

The amount of spent fuel in the repository is assumed to be in accordance with the SKB spent fuel reference scenario. The Data Report (SKB, 2010a, §3.1.6) states there is conceptual uncertainty in the accuracy of the reference scenario that can only be handled through sensitivity analysis, but no such discussion or analysis is presented in the Data Report or the Spent Fuel Report (SKB, 2010c). For example, there is no consideration of alternative fuel scenarios – what would be the impact on the spent fuel inventory if any nuclear power plants were to stop operations earlier or extend past the currently planned end date of 2045? It would be expected that SKB would need to consider the impact of a smaller or larger inventory on the design of the facility and in radiological dose assessments. In addition, there is no indication of the data precision in the inventories presented.

The data supplier recommends to the Data Report the nuclide half-life and specific activity data used in the Spent Fuel Report to produce the inventory data at the year 2045 (SKB, 2010a, Table 3-5; SKB, 2010c, Table C-1). These half-lives were used in the Origen-S calculations, although the Spent Fuel Report (SKB, 2010c, Table C-1) cites an unpublished SKB document so the original data source is unclear. However, the data supplier goes on to note (SKB, 2010a, §3.1.10) that, due to the current uncertainty over the half-lives of ^{108m}Ag and ^{79}Se in the scientific community, the half-life data provided in Table 3-5 of the Data Report "do not necessarily correspond to the data finally chosen for SR-Site". In fact, the SR-Site

Data Report Team goes on to recommend longer half-lives for these nuclides than those presented in the Spent Fuel Report, increasing the half-life from 127 years to 438 years for ^{108m}Ag and from $2.95x10^5$ years to $3.77x10^5$ years for ^{79}Se (SKB, 2010a, §3.1.11).

The difference in the proposed and accepted half-lives means that the inventory calculated in the Spent Fuel Report using the Origen-S code and the original data under-estimates the activity compared to if the longer half-lives recommended in the SR-Site Data Report were used; this difference is most significant at 2045 for ^{108m}Ag due do its shorter half-life. SKB (2010a, §3.1.11) acknowledges this inconsistency and judges it to be tolerable for ^{108m}Ag, but it is unclear why the spent fuel inventory was not simply re-calculated or the half-life data agreed for the SR-Site safety assessment before the inventory was calculated (particularly as the data sources for the revised half-lives date from 2004 and 2007 - Bienvenu *et al*. (2007) and Schrader (2004)). This indicates that the SR-Site Data Report was produced after the inventory calculations were complete. To further confuse matters, the SR-Site Data Team then goes on to use the original specific activity values for ^{108m}Ag and ^{79}Se when calculating the inventory in mol/canister for the 'average' canister (SKB, 2010a, Table 3-7) and the 'type' canisters (SKB, 2010a, Table 3-8).

Positively, the Radionuclide Transport Report (SKB, 2010i, Appendix E) cites the Data Report for the spent fuel inventory data, rather than the Spent Fuel Report (SKB, 2010c). However, as the inventory data are not reproduced in the Radionuclide Transport Report, the traceability and accuracy of data usage cannot be confirmed in this review.

The Radionuclide Transport Report (SKB, 2010i, Appendix E-1) notes that, after most of the calculations were completed, the inventory was corrected for all nuclides present in the PWR control rod clusters, resulting in a smaller corrected average inventory for all nuclides. The Radionuclide Transport Report states that the correction was performed completely in the Data Report (although there is no mention of this correction in the Data Report or the Spent Fuel Report) but that the correction was only applied for ^{108m}Ag in the radionuclide transport calculations (shear load case with early failure and in the additional cases to illustrate barrier function). No further corrections were implemented because the changes were considered by the authors of the Radionuclide Transport Report (SKB, 2010i, Appendix E-1) to be "either negligibly small or only affect nuclides with doses lower than [those] visible in the figures". SKB (2010i, Appendix E-1) notes that the changes for ^{113m}Cd (ratio between the corrected inventory and the old inventory of 0.252) and ^{93}Mo (0.855) are not negligible, but since the dose is lower than shown in the report figures the correction would not be visible in the reported results. The change for ^{108m}Ag (0.250) is only performed in the shear load case with early failure and in the additional cases to illustrate barrier function; for all other cases no change has been performed for the same reason as for ^{113m}Cd and ^{93}Mo. SKB (2010i, Appendix E-1) summarises that all results visible in the report figures and tables represent the corrected inventory, whereas the files archived at SKB are not corrected. Care must be taken by SKB that this inconsistency between reported and archived results does not lead to future confusion.

4.1.2. Solubility Data

Radioelement concentrations are used as the source term for the radionuclide transport calculations, and the concentrations depend on the solubility of the element and its chemical form. Element solubility limit values are required as an input to the radionuclide transport calculations. However, the solubility data section in the Data Report (SKB, 2010a, §3.4) does not present solubility limit values (although it does present the assumed solubility limiting phases), but thermodynamic data for a list of specified reactions in the form of equilibrium constants. These data are then input into the Simple Functions Spreadsheet Tool (Grivé *et al*., 2010a) in order to calculate the solubility limits, which are then input into the radionuclide transport calculations. Data traceability through the assessment was found to be the key issue associated with this data.

Tables 3-25 and 3-26 (SKB, 2010a) on sources of uncertainty in the data correctly cite Duro *et al*. (2006a), although they do not specify that the source is Table 5-1 in that report. Similarly, specific references are not provided for other tables in the Data Report, hindering traceability.

The recommended solubility limiting phases presented in Data Report Table 3-28 (SKB, 2010a) are stated to be sourced from Duro *et al*. (2006a), except for lead data from Grivé *et al*. (2010b). Table 8-1 (Duro *et al*., 2006a) in the recommended concentration limit section of the report does appear to supply the majority of the data for the Data Report table, but there are some differences. Some data appear to be taken from Table C-1 (Duro *et al*., 2006a) on solubility limits selected in Belgium (although one inaccuracy is that the limiting phase data are reported for solid $Sm(OH)_3$, not amorphous as stated) and some data are from Table C-5 on French solubility limits, but no statement is made as to the relevance or applicability of these data sources. However, the data sources for a number of phases have not been traced at all in the stated references, for example $Ca[SnO_6]$, $RaCO_3$(s), coffinite, schoepite, $CaUO_4$(s), $NaNpO_2CO_3$(s) and $PuCO_3OH$(s).

Two points are also observed in referencing in Duro *et al*. (2006a). The Forsmark reference groundwater composition in Table 3-1 (Duro *et al*., 2006a) is cited as an SKB personal communication, which is not transparent, although associated text on page 13 does note that the selected reference water corresponds to SICADA, code KFM02A sampled in Forsmark on 13th June 2003 packed in the interval 509-516.08 m. Secondly, Duro *et al*. (2006a) cites a report Duro *et al*. (2005) for supporting thermodynamic data, which is a 2005 Enviros report. However, an internet search suggests this report is actually a 2006 SKB report (TR-06-17), which is Duro *et al*. (2006b) in the SR-Site Data Report.

Figure 4.1 shows the results of an attempt by the authors of this report to trace the recommended equilibrium constant data presented in Tables 3-29 to 3-32 of the Data Report. No reference is given in the table captions for the data source so the seven reports listed as the main information sources in Table 3-22 (SKB, 2010a) were reviewed. As can be observed, the identified data sources appear to be Duro *et al.* (2006b), with Grivé *et al.* (2010b) for lead data, although a number of values are not consistent with the reference source. In the time available it was not possible to obtain and check the presented data against Hummel *et al*. (2002), the Nagra/PSI chemical thermodynamic database and one of the seven identified reports, and so it is assumed that where it was not possible to verify the data source, then the data derive from this report. It is recommended that this assumption and data source are checked in the Main Review Phase.

Figure 4.1: Annotated copies of SR-Site Data Report Tables 3-29 to 3-32 indicating the results of attempts to trace the original source reports (see text). Blue ink indicates data from Duro *et al*. (2006b) and red indicates data from Grivé *et al*. (2010b).

Table 3-29. Reactions and equilibrium constants recommended for use in the Simple Functions spreadsheet, valid at 25°C. (1/4).

Original sources for the stated values for equilibrium constants for the groundwater species and Sr were not found in this review.

	Species	Reaction		logK⁰	ΔlogK⁰	
Ra	$Ra(OH)^+$	$Ra^{2+} + H_2O = Ra(OH)^+ + H^+$		–13.50	0.25	
	$RaCO_3(aq)$	$Ra^{2+} + CO_3^{2-} = RaCO_3$	Duro 2006b Table 4-1	2.50 ✓	0.40	missing in 4-1
	$RaSO_4(aq)$	$Ra^{+2} + SO_4^{2-} = RaSO_4$	"	2.75 ✓	0.10	"
	$RaCl^+$	$Ra^{+2} + Cl^- = RaCl^+$		–0.10	0.30	
	$RaCO_3(s)$	$RaCO_3(s) = Ra^{2+} + CO_3^{2-}$	Table 4-1	–8.30 ✓	0.30	missing in 4-1
	$Ra(SO_4)(s)$	$Ra(SO_4)(s) = Ra^{2+} + SO_4^{2-}$	"	–10.26 ✓	0.09	"
Zr	$Zr(OH)_4(aq)$	$Zr^{4+} + 4H_2O = Zr(OH)_4(aq) + 4H^+$	Table 6-1 = −5.13 ± 0.36	–2.19 ✗	1.70 ✗	
	$Zr(OH)_4$(am,fresh)	$Zr(OH)_4(s) + 4H^+ = Zr^{4+} + 4H_2O$		–3.24	0.10	
	$Zr(OH)_4$(am,aged)	$Zr(OH)_4(s) + 4H^+ = Zr^{4+} + 4H_2O$	Grivé 2010b Table 2.2	–5.55 ✓	0.20 ✓	
Nb	$Nb(OH)_4^+$	$NbO_3^- + 2H^+ + H_2O = Nb(OH)_4^+$	Table 7-1	6.90 ✓	0.02 ✗	0.03
	$Nb(OH)_5(aq)$	$NbO_3^- + H^+ + 2H_2O = Nb(OH)_5(aq)$	"	7.34 ✓	0.02 ✗	0.03
	$Nb_2O_5(s)$	$Nb_2O_5(s) + H_2O = 2NbO_3^- + 2H^+$	"	–24.34 ✓	0.04 ✓	
Tc	TcO^{2+}	$TcO(OH)_2 + 2H^+ = TcO^{2+} + 2H_2O$		4.00	1.42	
	TcO_4^-	$TcO(OH)_2 + 0.75\ O_2 = TcO_4^- + 0.5\ H_2O + H^+$		32.94	2.05	
	$TcO(OH)^+$	$TcO(OH)_2 + H^+ = TcO(OH)^+ + H_2O$		2.50	0.30	
	$TcO(OH)_3^-$	$TcO(OH)_2 + H_2O = TcO(OH)_3^- + H^+$		–10.90	0.40	
	$Tc(CO_3)(OH)_2$	$TcO(OH)_2 + CO_3^{2-} + 2H^+ = Tc(CO_3)(OH)_2 + H_2O$		19.30	0.30	
	$Tc(OH)_3(CO_3)^-$	$TcO(OH)_2 + CO_3^{2-} + H^+ = Tc(OH)_3(CO_3)^-$		11.00	0.60	
	$TcO_2 \cdot 1.63H_2O$	$TcO_2\ 1.63H_2O = TcO(OH)_2 + 0.63\ H_2O$		–8.40	0.50	
Ni	$NiOH^+$	$Ni^{2+} + H_2O = NiOH^+ + H^+$	Table 9-3	–9.54 ✗	0.14 ✗	−9.50 ± 0.36
	$Ni(OH)_2(aq)$	$Ni^{2+} + 2H_2O = Ni(OH)_2(aq) + 2H^+$	"	–18.00 ✓	0.30 ✗	1.00
	$Ni(OH)_3^-$	$Ni^{2+} + 3H_2O = Ni(OH)_3^- + 3H^+$	"	–29.20 ✗	1.70 ✗	−29.70 ± 1.50
	$NiCl^+$	$Ni^{2+} + Cl^- = NiCl^+$	Table 9-10	0.08 ✗	0.60 ✗	1.00 ± 0.50
	$NiCO_3(aq)$	$Ni^{2+} + CO_3^{2-} = NiCO_3(aq)$	Table 9-5	4.20 ✗	0.40 ✗	4.00 ± 0.30
	$Ni(OH)_2(s)$	$Ni(OH)_2(s) + 2H^+ = Ni^{2+} + 2H_2O$	Table 9-3	11.03 ✗	0.28 ✗	10.50 ± 0.50
	$NiCO_3{:}5.5H_2O(s)$	$NiCO_3{:}5.5H_2O(cr) = Ni^{2+} + CO_3^{2-} + 5.5H_2O$		–7.52	0.24	
Pd	$Pd(OH)^+$	$Pd^{2+} + H_2O = Pd(OH)^+ + H^+$	Table 10-1	–1.86 ✓	0.30	Not stated in Table 10-1 (rows $Pd(OH)^+$ to $Pd(OH)_4^{2-}$)
	$Pd(OH)_2$	$Pd^{2+} + 2H_2O = Pd(OH)_2 + 2H^+$	"	–3.79 ✓	0.30	
	$Pd(OH)_3^-$	$Pd^{2+} + 3H_2O = Pd(OH)_3^- + 3H^+$	"	–15.93 ✓	0.30	
	$Pd(OH)_4^{2-}$	$Pd^{2+} + 4H_2O = Pd(OH)_4^{2-} + 4H^+$	"	–29.36 ✓	0.04	
	$PdCl^+$	$Pd^{2+} + Cl^- = PdCl^+$		5.10	0.01	
	$PdCl_2$	$Pd^{2+} + 2Cl^- = PdCl_2$		8.30	0.04	
	$PdCl_3^-$	$Pd^{2+} + 3Cl^- = PdCl_3^-$		10.90	0.07	
	$PdCl_4^{2-}$	$Pd^{2+} + 4Cl^- = PdCl_4^{2-}$		11.70	0.09	
	$Pd(OH)_2(s)$	$Pd(OH)_2(s) + 2H^+ = Pd^{2+} + 2H_2O$	§10.3.2	–1.61 ✓	1.16	Not stated.
Ag	$AgCl(aq)$	$Ag^+ + Cl^- = AgCl(aq)$	Table 11-6	3.27 ✓	0.17	Not stated in Table 11-6. (rows $AgCl(aq)$ to $AgCl_4^{3-}$)
	$AgCl_2^-$	$Ag^+ + 2Cl^- = AgCl_2^-$	"	5.27 ✓	0.37	
	$AgCl_3^{2-}$	$Ag^+ + 3Cl^- = AgCl_3^{2-}$	"	5.29 ✓	0.39	
	$AgCl_4^{3-}$	$Ag^+ + 4Cl^- = AgCl_4^{3-}$	"	5.51 ✓	1.71	
	AgOH (aq)	$H_2O + Ag^+ = AgOH + H^+$	Table 11-2	–12.00 ✓	0.30 ✓	
	$Ag(OH)_2^-$	$2H_2O + Ag^+ = Ag(OH)_2^- + 2H^+$	"	–24.00 ✓	0.10 ✓	
	$AgOH(s)$	$AgOH + H^+ = Ag^+ + H_2O$	"	6.30 ✓	0.05 ✓	
	$AgCl(cr)$	$AgCl(cr) = Ag^+ + Cl^-$ — Value for (s) not (cr)	Table 11-6	–9.75 ✓	0.04 ✓	

Figure 4.1: ***Continued.***

Table 3-30. Reactions and equilibrium constants recommended for use in the Simple Functions spreadsheet, valid at 25°C. (2/4)

	Species	Reaction	logK°	ΔlogK°	
Sn	$Sn(OH)^+$	$Sn^{4+} + 2H_2O = Sn(OH)^+ + 0.5O_2(g) + 3H^+$	–40.28	0.39	
	$Sn(OH)_2(aq)$	$Sn^{4+} + 3H_2O = Sn(OH)_2(aq) + 0.5O_2(g) + 4H^+$	–44.28	0.39	
	$Sn(OH)_4(aq)$	$Sn^{4+} + 4H_2O = Sn(OH)_4 + 4H^+$	–0.53	0.67	Table 4-4 ✓ ✓
	$Sn(OH)_5^-$	$Sn^{4+} + 5H_2O = Sn(OH)_5^- + 5H^+$	–8.53	0.73	" ✗ ✗ –8.50 ± 1.00
	$Sn(OH)_6^{2-}$	$Sn^{4+} + 6H_2O = Sn(OH)_6^{2-} + 6H^+$	–18.93	1.00	" ✓ ✓
	$SnO_2(am)$	$SnO_2(am) + 4H^+ = Sn^{4+} + 2H_2O$	–6.77	0.73	Table 4-5 ✓ ✓
	$Ca[Sn(OH)_6](s)$	$Ca[Sn(OH)_6](s) + 6H^+ = Sn^{4+} + 6H_2O + Ca^{2+}$	8.54	0.74	" ✓ ✓
Se	HSe^-	$SeO_4^{2-} + H^+ = HSe^- + 2O_2$	–84.61	0.44	
	SeO_3^{2-}	$SeO_4^{2-} = SeO_3^{2-} + 0.5O_2$	–13.50	0.34	
	Se^{2-}	$SeO_4^{2-} = Se^{2-} + 2O_2$	–99.52	0.77	
	H_2Se	$SeO_4^{2-} + 2H^+ = H_2Se + 2O_2$	–80.76	0.67	
	$HSeO_3^-$	$SeO_4^{2-} + H^+ = HSeO_3^- + 0.5O_2$	–5.15	0.41	
	H_2SeO_3	$SeO_4^{2-} + 2H^+ = H_2SeO_3 + 0.5O_2$	–2.51	0.43	
	$HSeO_4^-$	$SeO_4^{2-} + H^+ = HSeO_4^-$	1.75	0.10	Table 5-5 ✗ ✓ 1.80 ± 0.10
	$CaSeO_4$	$SeO_4^{2-} + Ca^{2+} = CaSeO_4$	2.00	0.10	Table 5-9 ✓ Not stated
	$FeSe_2(s)$	$FeSe_2(s) + 3.5O_2 + H_2O = 2SeO_4^{2-} + Fe^{2+} + 2H^+$	110.55	2.80	
	$Fe_{1.04}Se(s)$	$Fe_{1.04}Se(s) + 2.02O_2 + 0.08H^+ = SeO_4^{2-} + 1.04Fe^{2+} + 0.04H_2O$	82.87	0.92	
	$Se(s)$	$Se(s) + 1.5O_2 + H_2O = SeO_4^{2-} + 2H^+$	35.44	0.56	
Th	$Th(OH)^{3+}$	$Th^{4+} + H_2O = Th(OH)^{3+} + H^+$	–2.50	0.50	Table 14-1 ✗ ✗ –2.20 ± 0.20
	$Th(OH)_2^{2+}$	$Th^{4+} + 2H_2O = Th(OH)_2^{2+} + 2H^+$	–6.20	0.50	" ✗ ✗ –6.00 ± 0.60
	$Th(OH)_4$ (aq)	$Th^{4+} + 4H_2O = Th(OH)_4 + 4H^+$	–17.40	0.70	" ✗ ✗ –17.50 ± 0.50
	$Th(CO_3)(OH)_3^-$	$Th^{4+} + CO_3^{2-} + 3H_2O = Th(CO_3)(OH)_3^- + 3H^+$	–3.70	0.70	Grivé 2010b Table 2.3 ✓ ✓
	$Th(CO_3)(OH)_4^{2-}$	$Th^{4+} + CO_3^{2-} + 4H_2O = Th(CO_3)(OH)_4^{2-} + 4H^+$	–15.60	0.60	
	$Th(CO3)_5^{6-}$	$Th^{4+} + 5CO_3^{2-} = Th(CO_3)_5^{6-}$	31.00	0.70	
	$Th(OH)(CO_3)_4^{5-}$	$Th^{4+} + 4CO_3^{2-} + H_2O = Th(OH)(CO_3)_4^{5-} + H^+$	21.60	0.50	
	$Th(CO_3)_2(OH)_2^{2-}$	$Th^{4+} + 2CO_3^{2-} + 2H_2O = Th(CO_3)_2(OH)_2^{2-} + 2H^+$	8.80	0.50	
	$Th(SO_4)^{2+}$	$Th^{4+} + SO_4^{2-} = Th(SO_4)^{2+}$	6.17	0.32	Table 14-6 ✗ not stated 7.9
	$Th(SO_4)_2$ (aq)	$Th^{4+} + 2SO_4^{2-} = Th(SO_4)_2$	9.69	0.27	" ✗ not stated 11.8
	$Th(SO_4)_3^{2-}$	$Th^{4+} + 3SO_4^{2-} = Th(SO_4)_3^{2-}$	10.75	0.07	" ✗ not stated 12.7
	$ThCl^{3+}$	$Th^{4+} + Cl^- = ThCl^{3+}$	1.70	0.10	Table 14-7 ✗ not stated 1.21
	$ThO_2{\cdot}2H_2O$(am, aged)	$ThO_2{\cdot}2H_2O(am) + 4H^+ = Th^{4+} + 4H_2O$	8.50	0.90	Table 14-1 ✗
Pa	$PaO_2(OH)(aq)$	$PaO_2^+ + H_2O = PaO_2(OH)(aq) + H^+$	–4.50	0.20	Table 15-2 ✓ ✓
	$Pa_2O_5(s)$	$Pa_2O_5(s) + 2H^+ = 2PaO_2^+ + H_2O$	–4.00	1.00	" ✓ Not stated
U	UO_2OH^+	$UO_2^{2+} + H_2O = UO_2OH^+ + H^+$	–5.25	0.24	
	$UO_2(OH)_2(aq)$	$UO_2^{2+} + 2H_2O = UO_2(OH)_2(aq) + 2H^+$	–12.15	0.07	§16.2.1 ✓ not stated
	$UO_2(OH)_3^-$	$UO_2^{2+} + 3H_2O = UO_2(OH)_3^- + 3H^+$	–20.25	1.05	" ✓ not stated
	$UO_2(OH)_4^{2-}$	$UO_2^{2+} + 4H_2O = UO_2(OH)_4^{2-} + 4H^+$	–32.40	0.68	" ✓ not stated
	$(UO_2)_3(OH)_5^+$	$3UO_2^{2+} + 5H_2O = (UO_2)_3(OH)_5^+ + 5H^+$	–15.55	0.12	
	$(UO_2)_3(OH)_7^-$	$3UO_2^{2+} + 7H_2O = (UO_2)_3(OH)_7^- + 7H^+$	–32.20	0.80	§16.2.1 ✓ Not stated
	$UO_2CO_3(aq)$	$UO_2^{2+} + CO_3^{2-} = UO_2CO_3(aq)$	9.94	0.03	Table 16-3 ✓ ✓
	$UO_2(CO_3)_2^{2-}$	$UO_2^{2+} + 2CO_3^{2-} = UO_2(CO_3)_2^{2-}$	16.61	0.09	" ✓ ✓
	$UO_2(CO_3)_3^{4-}$	$UO_2^{2+} + 3CO_3^{2-} = UO_2(CO_3)_3^{4-}$	21.84	0.04	" ✓ ✓
	$(UO_2)_2CO_3(OH)_3^-$	$2UO_2^{2+} + CO_3^{2-} + 3H_2O = (UO_2)_2CO_3(OH)_3^- + 3H^+$	–0.86	0.50	" ✓ ✓
	UO_2^+	$UO_2^{2+} + 0.5H_2O = UO_2^+ + 0.25O_2 + H^+$	–19.30	0.02	
	$U(OH)_3^+$	$UO_2^{2+} + 2H_2O = U(OH)_3^+ + H^+ + 0.5O_2$	–37.22	1.00	
	$U(OH)_4(aq)$	$UO_2^{2+} + 3H_2O = U(OH)_4(aq) + 2H^+ + 0.5O_2$	–42.52	1.40	
	$U(CO_3)_4^{4-}$	$UO_2^{2+} + 4CO_3^{2-} + 2H^+ = U(CO_3)_4^{4-} + 0.5O_2 + H_2O$	2.60	0.93	
	$UO_2{\cdot}2H_2O(am)$	$UO_2{\cdot}2H_2O(am) + 2H^+ + 0.5O_2 = UO_2^{2+} + 3H_2O$	34.02	1.09	
	Coffinite	$USiO_4(s) + 2H^+ + 0.5O_2 + H_2O = UO_2^{2+} + H_4SiO_4$	31.02	6.57	
	Schoepite	$UO_3{\cdot}2H_2O(s) + 2H^+ = UO_2^{2+} + 3H_2O$	5.96	0.18	
	$CaU_2O_7{:}3H_2O(s)$	$CaU_2O_7{:}3H_2O + 6H^+ = 2UO_2^{2+} + Ca^{2+} + 6H_2O$	23.40	1.00	Grivé 2010b Table 2.4 ✓ ✓
	Becquerelite	$Ca(UO_2)_6O_4(OH)_6{\cdot}8H_2O + 14H^+ = Ca^{2+} + 6UO_2^{2+} + 18H_2O$	29.00	1.00	
	Uranophane	$Ca((UO_2)_2SiO_3OH)_2{\cdot}5aq + 6H^+ = Ca^{2+} + 2UO_2^{2+} + 2H_4SiO_4 + 5H_2O$	9.42	5.06	

Figure 4.1: *Continued.*

Table 3-31. Reactions and equilibrium constants recommended for use in the Simple Functions spreadsheet, valid at 25°C. (3/4)

	Species	Reaction		logK⁰	ΔlogK⁰
Np	$Np(OH)_3^+$	$Np^{4+} + 3H_2O = Np(OH)_3^+ + 3H^+$	Table 17-2	−2.80 ✓	1.00 ✓
	$Np(OH)_4$ (aq)	$Np^{4+} + 4H_2O = Np(OH)_4 + 4H^+$	"	−8.30 ✓	1.10 ✓
	$Np(CO_3)_4^{4-}$	$Np^{4+} + 4CO_3^{2-} = Np(CO_3)_4^{4-}$		36.68	1.03
	$Np(OH)_4(CO_3)^{2-}$	$Np^{4+} + CO_3^{2-} + 4H_2O = Np(OH)_4(CO_3)^{2-} + 4H^+$	Table 17-6	−6.83 ✓	1.13 ✓
	$NpCO_3(OH)_3^-$	$Np^{4+} + CO_3^{2-} + 3H_2O = NpCO_3(OH)_3^- + 3H^+$	"	3.82 ✓	1.13 ✓
	$Np(OH)_2(CO_3)_2^{2-}$	$Np^{4+} + 2CO_3^{2-} + 2H_2O = Np(OH)_2(CO_3)_2^{2-} + 2H^+$	"	15.17 ✓	1.50 ✓
	NpO_2^+	$Np^{4+} + 0.25O_2 + 1.5H_2O = NpO_2^+ + 3H^+$		10.57	0.12
	NpO_2OH	$Np^{4+} + 0.25O_2 + 2.5H_2O = NpO_2OH(aq) + 4H^+$		−0.73	0.71
	$NpO_2(OH)_2^-$	$Np^{4+} + 0.25O_2 + 3.5H_2O = NpO_2(OH)_2^- + 5H^+$		−13.03	0.51
	$NpO_2(CO_3)^-$	$Np^{4+} + 0.25O_2 + CO_3^{2-} + 1.5H_2O = NpO_2CO_3^- + 3H^+$		15.53	0.13
	$NpO_2(CO_3)_2^{3-}$	$Np^{4+} + 0.25O_2 + 2CO_3^{2-} + 1.5H_2O = NpO_2(CO_3)_2^{3-} + 3H^+$		17.10	0.16
	$NpO_2(OH)_2$	$Np^{4+} + 0.5O_2 + 3H_2O = NpO_2(OH)_2(aq) + 4H^+$		−0.45	1.51
	$NpO_2(CO_3)_2^{2-}$	$Np^{4+} + 0.5O_2 + H_2O + 2CO_3^{2-} = NpO_2(CO_3)_2^{2-} + 2H^+$		28.28	0.74
	$NpO_2(CO_3)_3^{4-}$	$Np^{4+} + 0.5O_2 + H_2O + 3CO_3^{2-} = NpO_2(CO_3)_3^{4-} + 2H^+$		31.13	0.24
	$NpO_2{\cdot}2H_2O$(am)	$NpO_2{\cdot}2H_2O(am) + 4H^+ = Np^{4+} + 4H_2O$		−0.70	0.50
	NpO_2OH (am, aged)	$NpO_2OH(am) + 4H^+ = Np^{4+} + 0.25\ O_2 + 2.5H_2O$		−5.87	0.23
	NpO2(CO3)Na·3.5aq	$NpO_2CO_3Na{\cdot}3.5H_2O + 3H^+ = Np^{4+} + 0.25O_2 + 5H_2O + CO_3^{2-} + Na^+$		−21.57	0.27
Pu	$PuOH^{2+}$	$Pu^{3+} + H_2O = PuOH^{2+} + H^+$		−6.90	0.30
	$Pu(OH)_2^+$	$Pu^{3+} + 2H_2O = Pu(OH)_2^+ + 2H^+$	Table 18-1	−15.90 ✓	1.00 ✓
	$Pu(OH)_3$(aq)	$Pu^{3+} + 3H_2O = Pu(OH)_3(aq) + 3H^+$	"	−25.30 ✓	1.50 ✓
	$PuCO_3^+$	$Pu^{3+} + CO_3^{2-} = PuCO_3^+$	Table 18-4	7.64 ✓	0.86 ✓
	$Pu(CO_3)_2^-$	$Pu^{3+} + 2CO_3^{2-} = Pu(CO_3)_2^-$	"	12.54 ✓	0.86 ✓
	$Pu(CO_3)_3^{3-}$	$Pu^{3+} + 3CO_3^{2-} = Pu(CO_3)_3^{3-}$	"	16.40 ✓	1.40 Not stated
	$PuSO_4^+$	$Pu^{3+} + SO_4^{2-} = PuSO_4^+$		3.91	0.66
	$Pu(SO_4)_2^-$	$Pu^{3+} + 2SO_4^{2-} = Pu(SO_4)_2^-$		5.70	0.91
	$Pu(OH)_3^+$	$Pu^{3+} + 0.25O_2 + 2.5H_2O = Pu(OH)_3^+ + 2H^+$		0.79	0.73
	$Pu(OH)_4$(aq)	$Pu^{3+} + 0.25O_2 + 3.5H_2O = Pu(OH)_4(aq) + 3H^+$		−5.41	0.84
	$Pu(CO_3)_4^{4-}$	$Pu^{3+} + 0.25O_2 + 4CO_3^{2-} + H^+ = Pu(CO_3)_4^{4-} + 0.5H_2O$		40.09	1.29
	PuO_2^+	$Pu^{3+} + 0.5O_2 + H_2O = PuO_2^+ + 2H^+$		6.42	0.96
	$PuO_2CO_3^-$	$Pu^{3+} + 0.5O_2 + CO_3^{2-} + H_2O = PuO_2CO_3^- + 2H^+$		11.54	0.97
	$PuO_2(OH)_2$(aq)	$Pu^{3+} + 0.75O_2 + 2.5H_2O = PuO_2(OH)_2(aq) + 3H^+$		−1.82	1.91
	PuO_2CO_3(aq)	$Pu^{3+} + 0.75O_2 + CO_3^{2-} + 0.5H_2O = PuO_2CO_3(aq) + H^+$		20.88	1.29
	$PuO_2(CO_3)_2^{2-}$	$Pu^{3+} + 0.75O_2 + 2CO_3^{2-} + 0.5H_2O = PuO_2(CO_3)_2^{2-} + H^+$		26.08	1.29
	$PuO_2(CO_3)_3^{4-}$	$Pu^{3+} + 0.75O_2 + 3CO_3^{2-} + 0.5H_2O = PuO_2(CO_3)_3^{4-} + H^+$		29.38	1.29
	$Pu(OH)_3$(s)	$Pu(OH)_3(cr) + 3H^+ = Pu^{3+} + 3H_2O$		15.80	1.50
	$PuCO_3OH$(s)	$PuCO_3OH(s) + H^+ = Pu^{3+} + CO_3^{2-} + H_2O$	Table 18-4	−5.94 ✗	1.26 not stated (−5.74)
	$Pu(OH)_4$(s)	$Pu(OH)_4(s) + 3H^+ = Pu^{3+} + 0.25O_2 + 3.5H_2O$		−3.89	1.47
	$PuO_2(OH)_2{:}H_2O$	$PuO_2(OH)_2{:}H_2O + 3H^+ = Pu^{3+} + 0.75O_2 + 3.5H_2O$		−5.85	1.55
Am	$Am(OH)^{2+}$	$Am^{3+} + H_2O = Am(OH)^{2+} + H^+$	Table 13-3	−7.20 ✓	0.50 ✓
	$Am(OH)_2^+$	$Am^{3+} + 2H_2O = Am(OH)_2^+ + 2H^+$	"	−15.10 ✓	0.70 ✓
	$Am(OH)_3$ (aq)	$Am^{3+} + 3H_2O = Am(OH)_3 + 3H^+$	"	−26.20 ✓	0.50 ✓
	$Am(CO_3)^+$	$Am^{3+} + CO_3^{2-} = Am(CO_3)^+$	§13.4.1	8.00 ✓	0.40 ✓
	$Am(CO_3)_2^-$	$Am^{3+} + 2CO_3^{2-} = Am(CO_3)_2^-$	"	12.90 ✓	0.60 ✓
	$Am(CO_3)_3^{3-}$	$Am^{3+} + 3CO_3^{2-} = Am(CO_3)_3^{3-}$	"	15.00 ✓	1.00 ✓
	$AmHCO_3^{2+}$	$Am^{3+} + H^+ + CO_3^{2-} = AmHCO_3^{2+}$	"	13.43 ✓	0.30 ✗ 0.55
	$Am(SO_4)^+$	$Am^{3+} + SO_4^{2-} = Am(SO_4)^+$	Table 13-10	3.30 ✓	0.15 ✓
	$Am(SO_4)_2^-$	$Am^{3+} + 2SO_4^{2-} = Am(SO_4)_2^-$	"	3.70 ✓	0.15 ✓
	$AmCl^{+2}$	$Am^{3+} + Cl^- = AmCl^{2+}$	Table 13-13	0.24 ✓	0.03 ✓
	$AmCl_2^+$	$Am^{3+} + 2Cl^- = AmCl_2^+$	"	−0.74 ✓	0.05 ✓
	$Am(OH)_3$ (am)	$Am(OH)_3(am) + 3H^+ = Am^{3+} + 3H_2O$	§13.3.2	16.90 ✓	0.80 ✓
	$Am(CO_3)(OH)$(~~s~~) cr	$Am(CO_3)(OH)(s) + H^+ = Am^{3+} + CO_3^{2-} + H_2O$	§13.4.1	−6.20 ✓	1.00 ✓
	Am2(CO3)3(s)	$Am_2(CO_3)_3(s) = 2Am^{3+} + 3CO_3^{2-}$	"	−33.40 ✓	2.20 ✓
	$Am(CO_3)_2Na{\cdot}5H_2O$(s)	$Am(CO_3)_2Na\ 5H_2O(s) = Am^{3+} + 2CO_3^{2-} + 5H_2O + Na^+$	"	−21.00 ✓	0.50 ✓
Cm	$Cm(OH)^{2+}$	$Cm^{3+} + H_2O = Cm(OH)^{2+} + H^+$	Table 13-3	−7.20 ✓	0.50 ✓
	$Cm(OH)_2^+$	$Cm^{3+} + 2H_2O = Cm(OH)_2^+ + 2H^+$	"	−15.10 ✓	0.70 ✓
	$Cm(OH)_3$	$Cm^{3+} + 3H_2O = Cm(OH)_3 + 3H^+$	"	−26.20 ✓	0.50 ✓
	$Cm(CO_3)^+$	$Cm^{3+} + CO_3^{2-} = Cm(CO_3)^+$	§13.4.1	8.00 ✓	0.40 ✓
	$Cm(CO_3)_2^-$	$Cm^{3+} + 2CO_3^{2-} = Cm(CO_3)_2^-$	"	12.90 ✓	0.60 ✓
	$Cm(CO_3)_3^{3-}$	$Cm^{3+} + 3CO_3^{2-} = Cm(CO_3)_3^{3-}$	"	15.00 ✓	1.00 ✓
	$CmHCO_3^{2+}$	$Cm^{3+} + H^+ + CO_3^{2-} = CmHCO_3^{2+}$	"	13.43 ✓	0.55 ✓
	$Cm(SO_4)^+$	$Cm^{3+} + SO_4^{2-} = Cm(SO_4)^+$	Table 13-10	3.30 ✓	0.15 ✓
	$Cm(SO_4)_2^-$	$Cm^{3+} + 2SO_4^{2-} = Cm(SO_4)_2^-$	"	3.70 ✓	0.15 ✓
	$CmCl^{2+}$	$Cm^{3+} + Cl^- = CmCl^{2+}$	Table 13-13	0.24 ✓	0.03 ✓
	$CmCl_2^+$	$Cm^{3+} + 2Cl^- = CmCl_2^+$	"	−0.74 ✓	0.05 ✓
	$Cm(OH)_3$ (am)	$Cm(OH)_3(am) + 3H^+ = Cm^{3+} + 3H_2O$	§13.3.2	16.90 ✓	0.80 ✓
	$Cm(CO_3)(OH)$(~~s~~) cr	$Cm(CO_3)(OH)(s) + H^+ = Cm^{3+} + CO_3^{2-} + H_2O$	§13.4.1	−6.20 ✓	1.00 ✓
	$Cm_2(CO_3)_3$(s)	$Cm_2(CO_3)_3(s) = 2Cm^{3+} + 3CO_3^{2-}$	"	−33.40 ✓	2.20 ✓

Duro 2006b states assumes same data for Cm as Am.

Figure 4.1: ***Continued.***

Table 3-32. Reactions and equilibrium constants recommended for use in the Simple Functions spreadsheet, valid at 25°C. (4/4)

	Species	Reaction		logK⁰	ΔlogK⁰	
Sm	$SmOH^{2+}$	$Sm^{3+} + H_2O = SmOH^{2+} + H^+$	Table 12-3	−7.90	0.10	
	$Sm(OH)_2^+$	$Sm^{3+} + 2H_2O = Sm(OH)_2^+ + 2H^+$	"	−16.50	0.20	
	$Sm(OH)_3$	$Sm^{3+} + 3H_2O = Sm(OH)_3 + 3H^+$	"	−25.90	1.00	
	$Sm(OH)_4^-$	$Sm^{3+} + 4H_2O = Sm(OH)_4^- + 4H^+$	"	−36.90	1.00	
	$SmCO_3^+$	$Sm^{3+} + CO_3^{2-} = SmCO_3^+$	Table 12-5	7.80	0.50	
	$Sm(CO_3)_2^-$	$Sm^{3+} + 2CO_3^{2-} = Sm(CO_3)_2^-$	"	12.80	0.60	
	$SmHCO_3^{2+}$	$Sm^{3+} + CO_3^{2-} + H^+ = SmHCO_3^{2+}$	"	12.43	0.50	
	$SmSO_4^+$	$Sm^{3+} + SO_4^{2-} = SmSO_4^+$	Table 12-10	3.50	0.20	
	$Sm(SO_4)_2^-$	$Sm^{3+} + 2SO_4^{2-} = Sm(SO_4)_2^-$	"	5.20	0.10	
	$SmCl^{2+}$	$Sm^{3+} + Cl^- = SmCl^{2+}$	Table 12-12	0.40	0.10	
	$Sm(OH)_3(am)$	$Sm(OH)_3(am) + 3H^+ = Sm^{3+} + 3H_2O$	Table 12-4	18.60	1.00	
	$Sm_2(CO_3)_3(s)$	$Sm_2(CO_3)_3(s) = 2Sm^{3+} + 3CO_3^{2-}$	Table 12-6	−34.50	2.00	
	$SmOHCO_3(s)$	$SmOHCO_3(s) + H^+ = Sm^{3+} + CO_3^{2-} + H_2O$	"	−7.70	0.30	Not stated
Ho	$HoOH^{2+}$	$Ho^{3+} + H_2O = HoOH^{2+} + H^+$	Table 12-3	−7.90	0.20	
	$Ho(OH)_2^+$	$Ho^{3+} + 2H_2O = Ho(OH)_2^+ + 2H^+$	"	−16.10	0.10	
	$Ho(OH)_3$	$Ho^{3+} + 3H_2O = Ho(OH)_3 + 3H^+$	"	−24.50	0.10	
	$Ho(OH)_4^-$	$Ho^{3+} + 4H_2O = Ho(OH)_4^- + 4H^+$	"	−33.40	0.20	
	$HoCO_3^+$	$Ho^{3+} + CO_3^{2-} = HoCO_3^+$	Table 12-5	8.00	0.40	
	$Ho(CO_3)_2^-$	$Ho^{3+} + 2CO_3^{2-} = Ho(CO_3)_2^-$	"	13.30	0.60	
	$HoHCO_3^{2+}$	$Ho^{3+} + CO_3^{2-} + H^+ = HoHCO_3^{2+}$	"	12.50	0.50	
	$HoSO_4^+$	$Ho^{3+} + SO_4^{2-} = HoSO_4^+$	Table 12-10	3.40	0.30	
	$Ho(SO_4)_2^-$	$Ho^{3+} + 2SO_4^{2-} = Ho(SO_4)_2^-$	"	4.90	0.30	Not stated
	$HoCl^{2+}$	$Ho^{3+} + Cl^- = HoCl^{2+}$	Table 12-12	0.30	0.50	
	$Ho(OH)_3(am)$	$Ho(OH)_3(am) + 3H^+ = Ho^{3+} + 3H_2O$	Table 12-4	17.80	0.30	Not stated
	$Ho_2(CO_3)_3(s)$	$Ho_2(CO_3)_3(s) = 2Ho^{3+} + 3CO_3^{2-}$	Table 12-6	−33.80	1.00	
Pb	$PbOH^+$	$Pb^{2+} + H_2O = PbOH^+ + H^+$	Grivé 2010b Table 2-1	−7.51	0.50	
	$Pb(OH)_2$ (aq)	$Pb^{2+} + 2\,H_2O = Pb(OH)_2 + 2\,H^+$	"	−16.95	0.20	
	$Pb(OH)_3^-$	$Pb^{2+} + 3\,H_2O = Pb(OH)_3^- + 3\,H^+$	"	−27.20	0.70	
	$Pb(OH)_4^{2-}$	$Pb^{2+} + 4\,H_2O = Pb(OH)_4^{2-} + 4\,H^+$	"	−38.90	0.80	
	$PbCO_3$ (aq)	$Pb^{2+} + CO_3^{2-} = PbCO_3$	"	7.00	0.50	
	$PbCl^+$	$Pb^{2+} + Cl^- = PbCl^+$	"	1.55	0.30	× 0.25
	$PbCl_2$	$Pb^{2+} + 2Cl^- = PbCl_2$	"	2.00	0.30	
	$PbCl_3^-$	$Pb^{2+} + 3Cl^- = PbCl_3^-$	"	2.01	0.30	× 0.50
	$PbClOH$ (s)	$PbClOH(s) + H^+ = Pb^{2+} + Cl^- + H_2O$	Table 2-2	0.62	0.30	Not stated
	$PbCO_3$ (Cerussite)	$PbCO_3\,(s) = Pb^{2+} + CO_3^{2-}$	"	−13.29	0.69	
	Hydrocerussite	$Pb_3(CO_3)_2(OH)_2 + 2\,H^+ = 3\,Pb^{2+} + 2\,CO_3^{2-} + 2\,H_2O$	"	−17.91	1.94	

In the review of the traceability of how the data recommended in the Data Report are used in the safety assessment, it is observed that the Data Report (SKB, 2010a, §3.4.1) states that Grivé *et al.* (2010a) use the thermodynamic data presented in the Simple Functions spreadsheet. However, Grivé *et al.* (2010a) does not cite the Data Report, but instead cites one of the source reports to the Data Report, Grivé *et al.* (2010b). As Grivé *et al.* (2010a) does not present the thermodynamic data built into the spreadsheet model, the data cannot be checked against the source without access to the Simple Functions spreadsheet. It is recommended this is reviewed in the Main Review Phase.

The Data Report (SKB, 2010a, §3.4.1) states that the output of the Simple Functions spreadsheet (calculated solubility limits using the specified thermodynamic data) is input to the SR-Site radionuclide transport modelling in COMP23 in order to assess the concentrations of dissolved radioelements inside the canister. The transport calculations are presented in the Radionuclide Transport Report (SKB, 2010i). Section F.1 (SKB, 2010i) states that the solubility limiting phases, reactions and equilibrium constants used in the Simple Functions spreadsheet are given in the Data Report (and accurately cites Tables 3-28 and 3-29), but the reporting by Grivé *et al.*

(2010a) on the Simple Functions spreadsheet does not cite the Data Report for its source data (as above).

Table F-1 (SKB, 2010i) records the filenames of archived groundwater composition files that contain the model input data used in the transport calculations. Such a table aids traceability and transparency, although it would be beneficial if the actual groundwater composition used in the calculations was reproduced in the report.

COMP23 does not allow changes in solubility limits with time and so SKB assumed a mixture of groundwater compositions to represent the entire time period was used to calculate one set of solubility limits (SKB, 2010i, §F.4). SKB argues that as the uncertainty in the thermodynamic data appears to have a larger impact on the solubility limits than the variations in the groundwater composition, a groundwater composition consisting of 25% of four different groundwater compositions (for temperate climate, permafrost climate, glacial climate and submerged climate) can be assumed. However, this assumption lacks a real physical basis and strong justification.

Table 3‑2 (SKB, 2010i) states that the solubility limits (the parameter CSOL) are "calculated distributions based on distributions of several groundwater compositions" but this does not clearly indicate that a single fixed groundwater composition was used, comprising an equal mixture of four climate compositions (as stated in Appendix F). The table also refers the reader to Section 3.4 of the Data Report for the solubility limit data but the Data Report provides equilibrium constant data that are input to the Simple Functions spreadsheet in order to calculate the solubility limit as a function of the specified groundwater composition.

A minor point is made that it is hard to assess the scale of data in Figure F-8 (SKB, 2010i) because only one value is given on the x-axis for all four charts presented.

Tables of the calculated solubility limits for each element are not presented in the Radionuclide Transport Report (SKB, 2010i); only graphical distributions are provided (Figures F-17 to F-28). It is unclear how these data have been input into COMP23, or what uncertainties and shape distributions have been assumed. This is not traceable and appears to require access to the model files in order to review data use.

Solubility limit data (without uncertainty values) are presented in Table 3-4 of the Radionuclide Transport Report (SKB, 2010i). However, the table caption states that the values are median values for temperate conditions. Yet, as discussed above, Appendix F states that the solubility values were calculated for a mixed temperate/permafrost/glacial/submerged groundwater composition. Therefore, these cannot be the actual data used in the transport model. It is also observed that the table does not present the solubility limit for the different recommended solubility limiting phases, or the phase to which the presented limits correspond. No statement is made to the effect that the bounding solubility limit for all the limiting phases is assumed.

Further, SKB (2010i, §3.7.3) states:

> "The solubility limits for plutonium are too high because of an incorrect value for the associated error in an equilibrium constant used in the calculations. Figures in Appendix F have been corrected but incorrect solubility limits for plutonium have been used in all calculation cases. No recalculations were made

since the fault was found at a very late stage of the SR-Site project, during the review of this report."

No mention of this error is made in Appendix F (SKB, 2010i), nor is it stated what the correct and incorrect equilibrium constant values are, whether the value is wrong or right in the Data Report, or what the error was due to – this error needs clarification in order to understand the issue further. Further, it is not understood how the figures in Appendix F have been corrected if the incorrect solubility limits have been used in all calculation cases.

The Simple Functions spreadsheet is regarded as a model in the Model Summary Report (SKB, 2010b, §3.20) so it unclear why the Simple Functions modelling step is not indicated as an input to COMP23 in the model linkage and data flow diagrams in the Radionuclide Transport Report (SKB, 2010i, Figures 3.2 and 3.3). In fact a word search shows that the Simple Functions tool is not mentioned at all in the main body of the Radionuclide Transport Report.

The above discussion finds that SR-Site does not include a traceable and unambiguous record of the input groundwater composition and the calculated solubility limits that are input to the radionuclide transport assessment. The source of the equilibrium constants presented in the Data Report is also unclear, with some inaccuracies in the data transfer, and without access to the Simple Functions spreadsheet it is not possible to check that the values in the Data Report are the ones actually used in the spreadsheet tool.

It is recommended that, considering the significance of solubility in the radionuclide transport calculations, solubility data are investigated in more detail in the Main Review Phase. The Radionuclide Transport Report (SKB, 2010i, §3.7.3) states that "used scripts, input data and main results are archived at SKB" and lists these unpublished documents in Table 3-8. By the document titles, two of these reports may contain a record of the solubility limit calculations and should be considered in the Main Review Phase:

- SKBdoc 1260107 version 1.0 "Supporting calculations related to radionuclide tramsport[sic]", SKB, 2010.
- SKBdoc 1260297 version 1.0 "Scripts and input data used for radionuclide transport calculations with COMP23", SKB, 2010.

The Model Summary Report (SKB, 2010b, §3.20.5) also cites (SKBdoc 1265616, Table 1-2) for data used in SR-Site that are archived at SKB, which may prove relevant.

4.2. Canister Data

4.2.1. Canister Geometry

As in the SR-Can safety assessment, the geometry of the spent fuel canisters is not presented in the Data Report. Previously (Hicks and Baldwin, 2008a, §3.1.1), canister geometry data were presented in the SR-Can Fuel and Canister Process Report. For SR-Site, canister dimension data for the reference canister are documented in the Canister Production Report (SKB, 2010d, §3.1.3), which in turn draws on (SKB, 2009a), an internal SKB document in Swedish that was not reviewed here.

The stated tolerance for some parameters in Tables 3-3 to 3-6 (SKB, 2010d) uses the terms h7, d8 and H8 without explanation; this terminology is not understood.

4.2.2. Copper Physical Data

In contrast to the previous review (Hicks and Baldwin, 2008, §3.1.2), the SR-Site Data Report does not discuss data for the canister thermal analysis. The Data Report (SKB, 2010a, p.28) states that the majority of the data concerning the canister, including dimensions, geometries and material data, are qualified in the Canister Production Report (SKB, 2010d).

The emissivity of the copper outer shell is required in order to determine the temperature at the canister-buffer interface when a gap exists between the canister and the buffer before the buffer material is fully saturated. In the previous review the SR-Can Data Report (SKB, 2006a, §4.1) indicated that an emissivity of 0.1 should be assumed based on laboratory measurements of a few canister lids used in welding experiments, but the source reference was not obtained in the previous review. Therefore, this parameter was reviewed again in SR-Site. However, this review found that the copper emissivity parameter is not easily traced.

The Canister Production Report (SKB, 2010d) makes no mention of copper emissivity. A value for copper emissivity of 0.020 is stated in the SR-Site Fuel and Canister Process Report (SKB, 2010g, §3.2), without reference, when calculating the temperature of the cast iron insert.

Hökmark *et al.* (2010) is referred to in the Canister Process Report (SKB, 2010g, §3.2) for discussion of the temperature distribution in the buffer/rock system, noting that the simplified calculations performed are based on pessimistic data for the copper surface temperature, copper emissivity and the size of the copper-iron gap. However, Hökmark *et al.* (2010) does not report an emissivity value; a search for "emissivity" in this report did not yield any results. It would aid traceability if, considering the length of the Hökmark *et al.* (2010) report, the relevant section or page was supplied in data citations.

Other SR-Site reports refer to Hökmark *et al.* (2009), which does discuss copper emissivity values. Hökmark *et al.* (2009, §3.3.3 and Appendix C) records that emissivity measurements were made by Uppsala University in 2003 on four copper lid samples from the Canister Laboratory, resulting in a mean measurement value of 0.0925.

With regard to the adequacy of references supporting the handling of canister thermal processes in SR-Site, the Canister Process Report (SKB, 2010g, §3.2) states that the supporting reference (Hökmark *et al.*, 2010) is an SKB report that has undergone a documented factual and quality review and that the simplified calculation performed is built on basic knowledge documented in books. It would build confidence if a reference was provided to documentation recording the review (an internal SKB document reference would be sufficient).

Hökmark *et al.* (2009) notes that the calculations performed therein verify that the reference gap effect (between the canister and buffer) is a reasonable estimate of the effects of a 10 mm uniform gap with a 0.1 copper surface emissivity. However, (Hökmark *et al.*, 2009, §3.3.3) also observes that: "One question, which will not be further addressed here, would be how the finish of the canister surface will change over time. If the surface finish tends to be more like ‘oxidized’ (e = 0.6 /CRC 1973/) or ‘new’ (e = 0.63 /Ageskog and Jansson 1999/) rather than between ‘polished’ (e = 0.023 /Cheremissinoff 1986/) and ‘calorized’ (e = 0.26 /CRC 1973/), after some years of exposure to the conditions in the deposition hole, this would increase the effective conductivity and reduce the temperature gap.” No indication is provided for where this question is addressed in SR-Site.

4.2.3. Initial Minimum Copper Thickness

The Data Report (SKB, 2010a, §4.1.10) presents ranges for the minimum copper thickness. For the whole surface of the copper shell, for normal operations after machining without defects, the minimum thickness is > 47.5 mm for > 99% of canisters, while a few canisters per thousand could be 45-47.5 mm thick. The fraction of canisters less than 45 mm thick is considered to be negligible. The data source cited is Table 7-3 in the Canister Production Report (SKB, 2010d); whilst the ranges presented in the Data Report are consistent, a footnote to Table 7-3 states that the probabilities associated with a minimum thickness of ≤ 47.5 mm occur only for disturbed operations considering both manufacturing processes and inspection. In addition, the probabilistic assessment is not traceably justified in the Canister Production Report (SKB, 2010d).

The reduction in copper shell thickness accounting for local reductions, including defects induced during hot-forming and welding, and surface damage induced during transportation, handling and deposition, is considered to be < 10 mm for > 99.9% of canisters (SKB, 2010d, Table 7-3; SKB, 2010a, §4.1.10). One canister per thousand may experience a reduction of 10-20 mm and a negligible number would be reduced by more than 20 mm (these values occur only for disturbed operations considering both manufacturing processes and inspection). This statement is well justified in Section 7.1.5 of the Canister Production Report, drawing on SKB’s testing of the proposed Friction Stir Welding (FSW) process, the pilot production of canisters and non-destructive testing (NDT), although it does rely on results in an unpublished internal SKB report (SKB, 2009c).

It is observed that for SR-Can all canisters sealed under normal operations were assumed to have a minimum thickness of 40 mm at the seal (Hicks and Baldwin, 2008, §3.1.3). For SR-Can it was assumed that 99% of the canisters would have a thickness of 40 to 50 mm at the weld and 1% would have a thickness of 35 to 40 mm. No mention is made in the SR-Site Data Report to explain this change. However, it is noted in the SR-Site Data Report (SKB, 2010a, §4.1.4) that the concept of an initial pinhole penetrating the copper shell has been abandoned in SR-Site due to improved welding methods (although this is considered as a hypothetical residual scenario later in the Data Report (SKB, 2010a, §4.2.4)).

Drawing on the above data, the data supplier (the Canister Production Report Team) in the Data Report (SKB, 2010a, §4.1.10) suggests that, building on experience from the pilot production of canisters, a copper thickness of 47 mm (rounded from the 47.5 mm given above for the welds) is used as a reference value in the corrosion calculations for the minimum thickness anywhere on the copper shell. In the data recommendation sub-section (SKB, 2010a, §4.1.12), the Data Report recommends use of the 47 mm value but also states that in corrosion evaluations in the safety assessment, the area exposed to corrosion and the number of canisters involved needs to be taken into account in an evaluation of whether the low probabilities of less than 47 mm copper thickness could influence the results.

It is observed that the recommended copper thickness of 47 mm is not discussed in the Canister Production Report (SKB, 2010d). The Data Report (SKB, 2010a, §4.1.1) cites (SKB, 2010h) for discussion of the SR-Site corrosion calculations to which the minimum copper thickness is an input. SKB (2010h) traceably uses the recommended minimum copper thickness, as discussed in Section 4.3.4 of that report and in Appendix 1 (it is noted that this appendix of data used in the calculations and identification of source references improves data traceability considerably).

The SR-Site Main Report (SKB, 2011a, §5.4) presents copper thickness data from Table 7-3 in the Canister Production Report (SKB, 2010d), whilst the minimum thickness value of 47 mm from the Data Report is referred to for the corrosion calculations in Section 10.4.9. It is observed in Section 5.4.3 (SKB, 2011a) that the initial state for the copper shell thickness deviates slightly from the design premise of a copper thickness of 5 cm but it was thought to be a sufficient input for further assessment of corrosion processes in SR-Site. The SR-Site Main Report (SKB, 2011a, §15.5.4) goes on to state that the current reference design is considered adequate, but it should be clarified that the lower limit for the manufactured thickness for the copper shell, bottom and lid, including tolerances, is 45 mm.

4.2.4. Canister Defect Evolution

The evolving canister defect discussion in the Data Report (SKB, 2010a, §4.2) concerns data needed in the safety assessment to model penetrating canister defects and radionuclide migration. Three canister failure modes are considered (postulated growing pinhole failure, corrosion and shear load) and three parameters are required to describe each failure mode:

- The defect radius r_{defect} (m). If the defect is so large that the canister offers no transport resistance, r_{defect} can be set as unlimited.
- The delay time t_{delay} (yr) between canister failure (penetrated copper shell) and the establishment of a continuous water pathway from the fuel to the canister exterior.
- The time t_{large} (yr) from repository closure to when r_{defect} is set to unlimited.

SKB (2010a, §4.2) states that the supplied data were produced by the SR-Site Data Report Team so no supplier formally exists. For the canister failure mode due to corrosion, t_{delay} is pessimistically set to zero and t_{large} is set to the time of failure. SKB (2010a, §4.2.3) states that because such a high degree of pessimism is used it is judged that these data do not need to be qualified. However, it should be explained why the decision has been taken to assume that as soon as the canister is penetrated a continuous water pathway with no transport resistance is established for the corrosion failure mode.

The growing pinhole failure mode is only used as a hypothetical residual scenario in SR-Site, in contrast to SR-Can, and draws upon SR-Can data, referring to the SR-Site Canister and Fuel Process Report (SKB, 2010g) and the SR-Can Data Report (SKB, 2006a, §4.4). A more specific reference to the SR-Site Canister and Fuel Process Report (SKB, 2010g) is not provided; a search for “pinhole” in the report presented no results, although Section 2.3 does discuss water processes following copper canister penetration and refers back to the SR-Site Data Report (Section 4.2) for discussion on the treatment of a developing penetrating defect in the copper shell. The SR-Can Data Report draws on Bond *et al.* (1997), data from which are categorised as supporting in the SR-Site Data Report (SKB, 2010a, Table 4-6), and Takase *et al*. (1999) and the SR 97 assessment.

Previous reviews of the SR-Can Data Report (Hicks and Baldwin, 2008, §3.1.5; Dverstorp and Strömberg, 2008, §11.10) found the selection of data unclear and SKB has revisited this during selection of the data for SR-Site. The explanation has been significantly improved, particularly for the justification of why a t_{delay} of 1,000 years is assumed for the pinhole failure mode and that it is pessimistic. Nonetheless, it is still assumed without explanation that the initial radius of the penetrating defect is 2 mm (SKB, 2010a, §4.2.5). The SR-Site Data Report (2010a, §4.2.5) does cite Bond *et al*. (1997) where it is estimated that corrosion consumes intruding water at a matching rate if the defect radius is at, or below, 1.62 mm; this may be a driver for the choice of a 2 mm defect aperture. Further, Coulson *et al*. (1990) is cited for dynamic viscosity values yet the report is not discussed in the section on document qualification (SKB, 2010a, §4.2.4).

A minor point, but it is observed that the Data Report Table 4-6 (SKB, 2010a) uses incorrect units of "m^2 m/s" for buffer hydraulic conductivity.

For canister failure due to shear load resulting in a circumferential crack, SKB (2010a, §4.2.7) calculates the delay time using a best estimate for the buffer hydraulic conductivity (5.1 x 10^{-14} m/s), the dynamic viscosity of water at 75°C, an assumed buffer thickness of 25 cm (reduced from the nominal initial thickness of 35 cm), and defect apertures of 1 mm and 10 mm. This gives rise to a delay time of the order of 100 years (147 years for the larger aperture and 252 years for the smaller aperture). SKB notes that in this case data uncertainty is over-shadowed by the degree of pessimism adopted in neglecting the hydrogen pressure build-up. It is noted that this calculation assumes a 10 cm shear, but as stated in Section 4.1.2 (SKB, 2010a), the criterion for maximum shear magnitude has been reduced from 10 cm in SR-Can to 5 cm in SR-Site; this adds to the pessimism in the delay time calculations but introduces an unexplained inconsistency in SKB's calculations. In addition, it is not explained why a 100 year delay time has been assumed for the canister shear failure mode yet zero delay is assumed for the canister corrosion failure mode.

In the SR-Can Data Report (SKB, 2006a, §4.4) it was expected that it would take at least 100,000 years from the time of the initial penetration before more extensive damage occurs, although a considerably smaller value of t_{large} could be argued if water flow in to the canister is assumed not to be hindered by hydrogen gas generation. This uncertainty was modelled in SR-Can as a right triangular distribution in log-space, with one year as the lower limit and 100,000 years as the upper limit and peak value. SKB (2010a, §4.2.7) states, without explanation, that only a single-point value is required for the SR-Site Data Report, so has calculated the arithmetic mean of the SR-Can distribution to be around 1.6 x 10^4 years, which is cautiously rounded to 1 x 10^4 years. However, it is unclear how this mean t_{large} value has been calculated for a distribution between one and 100,000 years.

Modelling of radionuclide release in the near-field is detailed in the Radionuclide Transport Report (SKB, 2010i). Table 3-2 in the Radionuclide Transport Report aids traceability considerably by listing the input data used for each canister failure scenario (consistently with the values published in the Data Report) and stating the relevant section of the Data Report.

4.3. Buffer and Backfill Data

4.3.1. Density and Porosity of Buffer and Backfill

The data supplier for buffer and backfill density and porosity data is not explicitly stated in the Data Report (SKB, 2010a, §5.1). However, as the buffer and backfill density data are taken from the Buffer and Backfill Production Reports (SKB, 2010e; 2010f), it is assumed that it is the SR-Site buffer and backfill production report teams that are the data suppliers for this section of the Data Report.

Regarding information sources, the Data Report (SKB, 2010a, §5.1.4) states that, as the data are qualified in the Buffer and Backfill Production Reports, only these reports are used to source data for the Data Report and that scrutiny of lower level references is part of the qualification process of the production reports. However, there is no discussion in the production reports of the qualified or supporting nature of the references drawn upon, or the nature of any review undertaken.

In addition, the original source reports for data in the Buffer Production Report are not always clearly indicated, for example the entire Section 4.2 (SKB, 2010e) on the initially installed buffer mass and density at saturation makes no reference to any report for the text, tables or figures. However, much of the data in this report derives from the Prototype Repository Experiment at the Äspö Hard Rock Laboratory and a key reference later in the Buffer Production Report appears to be Birgersson and Johannesson (2006). The cited report provides a brief statistical evaluation of the buffer density using results from the Prototype Repository Experiment.

Johannesson and Nilsson (2006) and Karnland *et al.* (2006) are two of the key references in the Backfill Production Report (SKB, 2010f), providing information on the composition and properties of Asha, Milos and MX-80 bentonite clays. Karnland *et al.* (2006) provides a detailed discussion of the relevant experiments and results. Johannesson and Nilsson (2006) investigates potential backfill mixtures in order to find the density of the materials required to fill the backfill design premise requirements - there is no target density in the design premises for backfill but the density is constrained by other design premises. For example, the backfill hydraulic conductivity must be less than 10^{-10} m/s and the swelling pressure greater than 0.1 MPa (SKB, 2011a, Figure 8-3; SKB, 2009b). The Johannesson and Nilsson (2006, §1) investigation assumed these values except that the requirement on swelling pressure was increased to 0.2 MPa, primarily because the relative influence of the friction in the oedometer is reduced at higher swelling pressures so a more accurate measurement can be made. This difference is not mentioned in the Backfill Production Report.

For both buffer and backfill densities, the data supplier is only required to provide density distribution information if the buffer/backfill cannot be produced and installed in such a way that the density conforms to the required design premises (SKB, 2010a, §5.1.1). It would be more logical if the data supplier, who is presumably more familiar with the data, was required to provide density distribution information whether or not the density conforms to the design premises, rather than the SR-Site Data Report team subsequently proposing a density distribution.

SKB (2010a, §5.1.1) gives the density of solid particles (grain density) as 2,780 kg/m^3 and cites Appendix A of both the Buffer Production Report and the

Backfill Production Report. This density is quoted in the relevant production report appendices but without reference, although Section 3.1.3 of the Buffer Production Report (SKB, 2010e) states that the saturated densities specified in the Design Premises Report are based on a grain density in the range of 2,750–2,780 kg/m^3, which SKB (2010e, §3.1.3) states, without support, is the grain density of many bentonite clays. However, the Design Premises Report (SKB, 2009b) does not state that the required buffer and backfill properties are based on such grain densities. Furthermore, items 3 and 6 in Table 5-2 of the Data Report (SKB, 2010a) incorrectly cite the dry density as 1,780 kg/m^3. A later statement in Section 6.1.1 of the Buffer Production Report (SKB, 2010e) cites Karnland (2010) for this grain density, which indeed does support this density on page 20, although it also goes on to state that a value of 2,750 kg/m^3 is used in the Buffer Production Report, which comes back to the original starting report but with a different value to that originally cited. Therefore, the grain density is not consistently and accurately reported in SR-Site.

In conjunction with this uncertainty, the SR-Site Data Report Team observes (SKB, 2010a, p.144) that an uncertainty interval of 2,750–2,780 kg/m^3 is "loosely" given for the density of the clay solids in the Buffer Production Report while 2,780 kg/m^3 is used as a single point value in the appendix calculations. The SR-Site Data Report Team also notes (SKB, 2010a, footnote 10) that if this value has been used to calculate the porosity then the resultant value of 0.466 should more properly have been rounded to 0.47 than 0.46; if 2,750 kg/m^3 has actually been used then a rounded porosity of 0.46 would be correct. However, while this uncertainty is acknowledged in the Data Report, the confusion is then ignored.

The Data Report states (SKB, 2010a, §5.1.11) that, in the calculations the SR-Site Data Report Team performed, a grain density of 2,780 kg/m^3 and water density of 1,000 kg/m^3 was assumed. Table 4.1 below records the original data supplied to the Data Report from the relevant Production Reports, the SR-Site Data Report Team results for the corresponding porosity and dry/saturated density, and then the same calculations performed by the authors of this review. Whilst the SR-Site team itself acknowledges rounding discrepancies in the supplied buffer and backfill porosities (SKB, 2010a, footnote 10 and p.145), these are accepted. However, as observed in Table 4.1, a further small discrepancy or typographical mistake has been incorporated in the buffer porosity (43.5% compared with 43.8%) and there appears to be an inexplicable discrepancy between the calculated saturated backfill density of 1,921 kg/m^3 by the SR-Site Team compared with a value of 1,934 kg/m^3 calculated in this review. However, these discrepancies are unlikely to have a noticeable impact on the safety assessment; this is particularly true because none of the SR-Site reports considered in this review were found to cite use of this data (see following text).

Table 4.1: Buffer and backfill density and porosity data in the SR-Site Data Report (from SKB, 2010a, Sections 5.1.10-5.1.12), and data check calculations performed in this review. The buffer saturated and backfill dry densities were supplied from the relevant Production Report (SKB, 2010e and 2010f) and the SR-Site Data Report Team calculated the corresponding dry/saturated densities using Equations 5-1 and 5-2 in the Data Report (SKB, 2010a) and assuming a grain density of 2,780 kg/m^3 and a water density of 1,000 kg/m^3. The Data Report calculations are performed again here as part of this review using the same equations and data assumptions. Values in bold indicate a difference in the calculated value by this review from those presented in the Data Report (SKB, 2010a, Tables 5-5 and 5-6).

Data Supplier		SR-Site Data Report Team		This Review	
Buffer					
Saturated Density (kg/m^3)	Porosity (-)	Dry Density (kg/m^3)	Porosity (%)	Dry Density (kg/m^3)	Porosity (%)
1,950	0.46	1,484	46*	1,484	47*
2,000		1,562	43.5	1,562	43.8
2,050	0.41	1,640	41	1,640	41
Backfill					
Dry Density (kg/m^3)	Porosity (-)	Saturated Density (kg/m^3)	Porosity (%)	Saturated Density (kg/m^3)	Porosity (%)
1,458	0.48	1,921	48	1,934	48
1,504	0.46	1,963	46	1,963	46
1,535	0.44	1,983	44†	1,983	45†

* SKB (2010a, footnote 10) acknowledges the buffer porosity should be rounded to 47% if the grain density is 2,780 kg/m^3, but the value is left at 46% as supplied.

† SKB (2010a, p.145) acknowledges the "odd" buffer porosity rounding if the grain density is 2,780 kg/m^3, but the value is accepted as 44%.

In review of the traceability of how the Data Report recommended data are used in the safety assessment, it is observed that the Data Report (SKB, 2010a, §5.1.1) states that "the buffer and backfill porosities and densities delivered in this section will be used in a number of SR-Site modelling activities, including THM modelling, hydrogeological modelling, and modelling of buffer erosion". The following four reports are cited in the Data Report but, as described below, no density and porosity data was found to derive from the Data Report:

- The THM modelling performed is described in Åkesson *et al*. (2010a; 2010b). Review of Åkesson *et al*. (2010a) found it to be a data report created as a supplement to the main SR-Site Data Report, with the text prepared in agreement with the SKB quality assurance instruction "Supplying data for the SR-Site data report". No data in the report appear to derive from the main SR-Site Data Report or the Buffer and Backfill Production Reports, although the original reports cited in the Production Reports are cited, e.g., Karnland *et al*. (2006) and Johannesson and Nilsson (2006). Review of Åkesson *et al*. (2010b) found that it does not cite the SR-Site Data Report, only the Buffer and Backfill Production Reports and the supplementary data report of Åkesson *et al*. (2010a).

- The hydrogeological modelling is summarised by Selroos and Follin (2010), but review of this report found that it does not appear to cite density and porosity values. It is observed that this report appears to generally provide good referencing to specific sections and tables within the citations.
- The erosion modelling is described in Neretnieks *et al*. (2009). This report was published over a year before the SR-Site Data Report was published and does not cite it.

Looking more widely among the SR-Site reports, the Buffer and Backfill Process Report (SKB, 2010j) cites the data source for its Table 2-5 as the Backfill Production Report (SKB, 2010f), rather than the Data Report, and it also does not provide a more specific reference. Further, Section 2.2.2 (SKB, 2010j) cites the Buffer Production Report (SKB, 2010e) for initial variable values, rather than the Data Report. In addition, a more specific reference should be provided and it would aid traceability if the values of the initial variables referred to were reproduced in the Buffer and Backfill Process Report. Similarly, Section 2.3.2 (SKB, 2010j) also cites the Backfill Production Report (SKB, 2010f) rather than the Data Report for initial variable values, again without a more specific reference within the Production Report. The Process Report does not appear to cite the Data Report for any buffer/backfill density and porosity values.

Regarding the adequacy of references supporting the suggested handling in the safety assessment, an analysis in the Buffer and Backfill Process Report (SKB, 2010j, p.229) states that "All the references in this section are from peer reviewed scientific journals". Such a statement may support an assessment of the quality of the cited documents but consideration should also be given to the relevance of the references to a KBS-3 repository and the validity of data use in this context.

The SR-Site Main Report (SKB, 2011a) also does not provide specific section or table numbers in its citations, hindering data traceability. Section 5.5 (SKB, 2011a) contains a number of tables from the Buffer Production Report but does not state the data source in the table captions, although there are general statements in surrounding text referring to the Buffer Production Report. Similarly, the text in Section 5.6 (SKB, 2011a) refers to the Backfill Production Report, not the Data Report.

From the above, it appears that buffer and backfill density and porosity data used in the safety assessment are not sourced from the SR-Site Data Report.

4.4. Geosphere Data

4.4.1. Flow Related Migration Properties

Several parameters controlling radionuclide transport are related to the amount and distribution of groundwater flow. The values of these flow-related migration parameters were obtained by SKB using numerical simulation of groundwater flow and are described in Section 6.7 of the Data Report (SKB, 2010a). The parameters requested of the data supplier for each deposition hole are the Darcy flux (q), the equivalent flow rate (Q_{eq}), advective travel time (t_w), and flow-related transport resistance (F) for each of three release pathways (Q1, Q2 and Q3). Additional parameters requested are longitudinal dispersivity (a_L) along the flow path, Péclet number (P_e) and maximum penetration depth for solute diffusion into the rock matrix (L_D).

The data presented in the Data Report (SKB, 2010a, §6.7) are supplied by the SR-Site Data Report Team, so no supplier formally exists. The data are not sorted into qualified and supporting for this section of the Data Report because the presented data are outputs from the SR-Site hydrogeological modelling, the inputs for which are qualified in other sections of the data report (primarily Section 6.6).

A good discussion of the various sources of uncertainty (conceptual, precision, bias, representativity, spatial and temporal) is presented in Sections 6.7.6 to 6.7.8 (SKB, 2010a). SKB (2010a, §6.7.7) states that "it is not possible to provide detailed quantitative measures of the uncertainties listed" but does judge that the greatest uncertainty is associated with the periglacial/glacial model, and then with the performance measures associated with the temperate model. It is recognised that uncertainty in these parameters has a different character to that in other parameters because the climate change parameters are not directly measureable. However, it would be helpful if an indication could be given of the magnitude of uncertainty associated with the modelling undertaken to produce climate parameters.

Tables 6-80 and 6-81 (SKB, 2010a) present statistics of the Darcy flux and flow-related transport resistance for the temperate period at 2000 AD and for the glacial case without permafrost for an ice front location directly above the repository. The data source for both tables is not provided, and the two reports cited as the main data sources for this section of the Data Report do not include these tables (Joyce *et al.* (2010) and Vidstrand *et al.* (2010)). In addition, for the q(Q1) parameter in Table 6-80, the minimum and maximum values are stated as -8.61 and -7.64, respectively. However, the 5th and 95th percentile values are stated as -7.17 and -3.73, respectively, indicating that the maximum value should be greater than -3.73. Similarly, no source is provided for the data in Table 6-83 or Figure 6-67 (although the latter may well be reproduced from Joyce *et al.* (2010, Figures 6-8 and 6-9)).

SKB (2010a, §6.7.9) recognises that flow path characteristics in terms of length and discharge locations will vary between different climatic states and then makes the assumption that these different characteristics are of second order relative to the changes implied by the change in flow magnitude. Without further discussion to support this assumption or reference to arguments in an external document it cannot be determined whether this assumption is valid.

The SKB instruction for supplying data to the Data Report allows that, where it is impractical to tabulate data in the Data Report (e.g., where there are many thousands of data points), it is sufficient to precisely refer to a database or equivalent (SKB, 2010a, §2.3.10). Flow-path data are not presented in Section 6.7 (SKB, 2010a) but Tables 6-82 and 6-84 list the hydrogeological modelling cases and the unpublished SKB documents that are said to contain the equivalent flow rate, advective travel time and flow-related transport resistance data that are used in the models (SKBdoc 1255039 and SKBdoc 1256019, although the precise report data tables are not cited). It is recommended that SSM requests these documents from SKB and reviews the data, their traceability and application in the hydrogeological modelling in the Main Review Phase.

The suggested Péclet number, longitudinal dispersivity and maximum penetration depth are discussed at the end of Section 6.7.10 and the recommended single-point values are presented in Table 6-85. SKB (2010a, §6.7.10) argues that field evidence from tracer tests suggests that the dispersion length is typically 10% of the distance of a tracer test, hence leading to a Péclet number of 10, but no reference is cited to support this statement. However, the recommended parameter values (Péclet number of 10, dispersivity of 50 m and penetration depth of 12.5 m) for use in hydrogeological modelling are traceably presented in the Radionuclide Transport Report (SKB, 2010i, Table 3-2).

4.5. Summary

The Data Report is one of the series of SR-Site safety assessment reports and from the report title it would be anticipated that the Data Report would provide the primary source of data for the safety assessment. Further, it would be expected that other reports in the safety assessment series would refer to relevant sections of the Data Report when analysing specific processes and scenarios, and that the Data Report would cross-refer to the relevant analysis in the safety assessment documentation. However, many of the SR-Site reports appear to contain comprehensive discussions of data relating to relevant processes and these reports do not always make use of the material presented in the Data Report. In general, the approach to documenting data and parameters relating to specific processes appears to be inconsistent throughout SR-Site and, as a result, some of the discussion in the Data Report appears superfluous.

The main findings from this review of selected data sets are as follows:

- Efforts have been made to separate the views of the SR-Site Data Report Team from those of the experts authoring the supporting documents. This has generally been successful, although it is not always clear who the actual data supplier is.
- It was recommended in the review of the SR-Can Data Report that more specific referencing was included in citations, for example to relevant sub-sections of reports or tables. This has been applied in a large proportion of the discussions reviewed in the SR-Site Data Report, which has aided traceability. However, the majority of the SR-Site reports do not include specific referencing and so when trying to trace data outside the Data Report traceability is hindered.
- Where data are qualified outside the Data Report, the scrutiny of lower level references is considered to be part of the qualification process of that report. However, typically there is no discussion in those reports of the qualified or supporting nature of the references drawn upon, or the nature of any review undertaken (e.g. the spent fuel inventory is qualified in the Spent Fuel Report (SKB, 2010c) and bentonite density and porosity are qualified in the Buffer and Backfill production Reports (SKB, 2010e; 2010f)). It is also unclear if any attempt is made to qualify the data to the requirements specified in the QA instruction “Supplying data to the SR-Site Data Report”.
- A number of unpublished reports have been identified that are key to the SR-Site safety assessment; it is recommended that these are reviewed in the Main Review Phase.
- Some of the parameters reviewed are more traceably documented than others. Element solubility values are particularly difficult to trace and are not well referenced, as are flow-related migration properties. An element

of educated guess-work and word searches in documents is often required to correctly identify original source reports.

- A number of instances of errors introduced when transferring data between reports have been identified, e.g., for element equilibrium constants, bentonite densities and porosities, and flow-related migration properties. This particularly applies to uncertainty values, where less care appears to have been applied than for the central value.
- It is unclear where the question raised by Hökmark *et al*. (2009, §3.3.3) is addressed on how the copper canister surface finish (and therefore its emissivity value) will change over time.
- A number of updates and errors have been identified by SKB at a late stage in the assessment (e.g., a revised PWR control rod cluster inventory, revised nuclide half-lives, and errors in the plutonium equilibrium constant). It is often unclear which reports have been updated to account for this and which have not; the corrections do not appear to have been implemented across all of the SR-Site reports.
- In some cases assumptions made and calculations performed are not supported by sufficient explanation in the Data Report to enable the reader to understand and/or feel the case is made, e.g., how the mean t_{large} value for the pinhole corrosion case is calculated, or why it can be assumed that different flow path characteristic uncertainties are of second-order importance compared to those implied by changes in flow magnitude.
- The Data Report does not always provide clear information on how and where data are used in the SR-Site assessment, which makes the task of checking the traceability of information through the assessment difficult, although it is noted that this has been improved since SR-Can.
- Reports using data presented in the Data Report do not consistently refer to the Data Report itself, but often to the original report supplying data to the Data Report. This again indicates that the Data Report has been produced late in development of SR-Site, rather than at the start of the assessment.

Although the data errors identified in this selective review are unlikely to be of such significance that they affect the calculations and arguments presented in the safety case, the number of such simple and avoidable errors and lack of traceability raises concerns that there could be significant undetected errors elsewhere.

Investigation of reports not obtained during this review, which support the selected data sets considered here, are recommended for review in the Main Review Phase, e.g., unpublished reports supplying the original spent fuel inventory data, reporting results of solubility limiting values and files of flow-related migration data. It is also recommended that the traceability and accuracy of other parameters not considered here are reviewed in the Main Review Phase, particularly parameters from the Surface System Data chapter, which has not been considered. Further, it is recommended that parameters qualified in reports other than the Data Report are reviewed, especially as it is not clear that such data are subject to any specific data QA procedure.

5. Summary and Conclusions

On 16th March 2011SKB applied for a licence to construct and operate a spent nuclear fuel encapsulation facility in Oskarshamn Municipality and a final repository for the encapsulated fuel at Forsmark in Östhammar Municipality. SKB's SR-Site safety assessment for the spent fuel repository is currently being reviewed by SSM and its external experts in the first step of the review, the Initial Review Phase. This report provides a review of quality assurance requirements, data documentation and traceability in the SR-Site safety assessment.

The review has been carried out in three parts. First, the SR-Site QA plan and project steering documents were reviewed. Secondly, the SR-Site Data Report was reviewed, focusing on its stated objectives, structure and data selection. Finally, spot-checks of selected data sets were performed, considering data traceability in the SR-Site safety assessment.

Twelve QA documents were reviewed in this work. Overall, the reviewed QA instructions do provide reasonably comprehensive coverage of quality-affecting issues relating to the SR-Site safety assessment and, if implemented correctly, will generate confidence in the reliability of the safety assessment results. However, progress in development of the QA documents and instructions has been ongoing during production of the safety assessment SR-Site, possibly hindering full application of the QA procedures and opportunities for any comprehensive QA audits of the SR-Site project.

A number of review comments have been made during this review but key points are summarised below.

- The revised SR-Site QA plan states that an internal QA audit was ordered by the SR-Site project to be held during the first half of 2009, but there is no indication that the audit took place, despite the QA plan dating from July 2009. It should be clarified with SKB if the audit took place, what the findings were and if there were any non-conformities to be addressed.
- It is unclear if those calculations not subject to the Instruction for Model and Data QA are subject to any specific QA procedure, particularly if such calculations are not documented in the assessment reports. It should be verified that these calculations have been independently checked.
- SKB does not require codes used and owned by contractors to be stored in the centralised model storage system. It should be clarified how SKB ensures that it has access to the models used in the assessments and that it is not overly dependent on a single contractor for these models. Further, it is unclear if SKB independently audits the models used by contractors.
- A key concern in this review is that the QA instruction on supplying data to the SR-Site Data Report was revised after the report was published (Version 4.0 is dated May 2011 yet the SR-Site Data Report was published in December 2010). The comments in the procedure revision history note that the responsibility for data qualification approval has been redefined and that a number of demands on the supplier and/or customer have been softened to reflect the Data Report content. This implies that the supply of data to the Data Report did not follow the requirements set out in the

procedure and that the procedure was altered subsequently to reflect what did take place. The QA instruction for the supply of data to the SR-Site Data Report should be a relatively static procedural reference, possibly subject to revision during the course of the project, but should not require revision following completion of the activity for which it was written. It is not clear which parameters were produced to the original, more stringent, procedure and for which parameters the revised procedure was required. This requires clarification from SKB.

The SR-Site Data Report aims to compile, document and qualify input data identified as essential for the long-term safety of a KBS-3 repository. The process followed to identify the essential data is clearly defined, making use of the Assessment Model Flowcharts and by identifying input parameters to the COMP23 and FARF31 computational codes. However, there is no discussion of the criteria that the SR-Site Data Report Team used to determine which data to include in the Data Report, or who made the decision and where it is recorded. It would aid traceability if a central list of all the data reviewed by the SR-Site Data Report Team had been produced, noting whether the data were determined to be sufficiently significant to include in the Data Report or not.

Further, as not all data identified as essential are qualified and presented in the Data Report, it is often difficult to find where in the suite of SR-Site documents a specific parameter is presented, or even if the data are qualified at all. Without a reference table recording in which report each parameter is qualified (or is not regarded as essential and is therefore not qualified at all), it is necessary to search a number of reports to find the data qualification for a specific parameter. In addition, it should be clarified whether data not included in the Data Report, whether regarded as essential or not, are subject to any QA requirements (other than general review of the report in which it is presented). As defined in the SR-Site QA documentation, only data regarded as essential and presented in the Data Report appear to be covered by specific data QA requirements.

The traceability of selected data sets in the SR-Site Data Report was examined through spot-checks and examination of lower level references. From the report title it would be anticipated that the Data Report would provide the primary source of data for the safety assessment. Further, it would be expected that other reports in the safety assessment series would refer to relevant sections of the Data Report when analysing specific processes and scenarios, and that the Data Report would cross-refer to the relevant analysis in the safety assessment documentation. However, many of the SR-Site reports appear to contain comprehensive discussions of data relating to relevant processes and these reports do not always make use of the material presented in the Data Report. In general, the approach to documenting data and parameters relating to specific processes appears to be inconsistent throughout SR-Site and, as a result, some of the discussion in the Data Report appears superfluous.

Key findings from the review of selected data sets are as follows:

- It was recommended in the review of the SR-Can Data Report that more specific referencing was included in citations, for example to relevant sub-sections of reports or tables. This has been applied in a large proportion of the discussions reviewed in the SR-Site Data Report, which has aided traceability. However, the majority of the SR-Site reports do not include specific referencing and so when trying to trace data outside the Data Report traceability is hindered.

- Where data are qualified outside the Data Report, the scrutiny of lower level references is considered to be part of the qualification process of that report. However, typically there is no discussion in those reports of the qualified or supporting nature of the references drawn upon, or the nature of any review undertaken.
- Some of the parameters reviewed are more traceably documented than others. Element solubility values are particularly difficult to trace and are not well referenced, as are flow-related migration properties. An element of educated guess-work and word searches in documents is often required to correctly identify original source reports.
- Instances of errors introduced when transferring data between reports have been identified, e.g., for element equilibrium constants, bentonite densities and porosities, and flow-related migration properties.
- A number of updates and errors have been identified at a late stage in the assessment (e.g., a revised PWR control rod cluster inventory, revised nuclide half-lives, and errors in the plutonium equilibrium constant). It is often unclear which reports have been updated to account for this and which have not; the corrections do not appear to have been implemented across all the SR-Site reports.
- In some cases, assumptions made and calculations performed are not supported by sufficient explanation in the Data Report to enable the reader to understand and/or feel the case is made, e.g., how the mean t_{large} value for the pinhole corrosion case is calculated, or why it can be assumed that different flow path characteristic uncertainties are of second-order importance compared to those implied by changes in flow magnitude.
- The Data Report does not always provide clear information on how and where data are used in the SR-Site assessment, which makes the task of checking the traceability of information through the assessment difficult, although it is noted that this has been improved since SR-Can.
- Reports using data presented in the Data Report do not consistently refer to the Data Report itself, but often to the original report supplying data to the Data Report. This again indicates the Data Report has been produced late in development of SR-Site, rather than at the start of the assessment.

Although the data errors identified in this selective review are unlikely to be of such significance that they affect the calculations and arguments presented in the safety case, the number of such simple and avoidable errors and lack of traceability raises concerns that there could be significant undetected errors elsewhere.

The key conclusion of this review is that the Data Report appears to not be quite one thing or another – it is expected that a safety assessment data report would be the reference document for all data used in the assessment, but that is not the case, and not all the parameters presented are fully qualified in the Data Report. Some data are qualified in the Data Report, some data are qualified in other reports, and data regarded as unessential for the assessment are not qualified and centrally recorded at all. Further, some assessment reports cite the Data Report and some cite other SR-Site reports; the Data Report is not consistently the key source. Considering the way in which the SR-Site Data Report has been developed and applied, as compared with expectations for a safety assessment database, the reviewers question the usefulness of the Data Report.

A number of recommendations have been made in the text above for clarifications to be sought from SKB in the Main Review Phase. The appendices list all clarification questions and recommended topics for the Main Review Phase. In general, it is recommended that the reports not obtained during this review of selected parameters are investigated and that the traceability and accuracy of other parameters not considered here are reviewed. Further, it is recommended that parameters qualified in reports other than the Data Report are reviewed, especially as it is not clear that such data are subject to any specific data QA procedure.

6. References

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APPENDIX 1

Coverage of SKB Reports

Report sections considered in this review are listed in the table below. Due to the nature of this review task (traceability of data through the SR-Site application), a large number of SKB reports has been accessed but the cited text has generally been reviewed at a high-level focused on a particular parameter.

Table A1:1

Reviewed report	Reviewed sections	Comments
TR-11-01, Long-term safety for the final repository for spent nuclear fuel at Forsmark, Main report of the SR-Site Project	Sections 1-3, 5, 8, 9, 15	
TR-10-52, SR-Site Data Report	Sections 1, 2, 3.1, 3.4, 4, 5.1, 6.6 (part), 6.7	
SR-Site QA-related documents (SKBdoc 1174832, 1064228, 1082126, 1082127, 1082128, 1082130, 1082129, 1183027, 1186612, 1186579, 1182953, 1096716)	All sections	Full document titles and versions recorded in Table 2.1.
TR-06-25, SR-Can Data Report	Brief revision of previously analysed parameters	
TR-09-22, Design Premises for a KBS-3V Repository Based on Results From the Safety Assessment SR-Can and Some Subsequent Analyses	Section 2 (part)	
TR-10-14, Canister Production Report	Sections 1, 2, 3, 4, 5, 6 (part), 7, Appendices A & B	
TR-10-46, Fuel and Canister Process Report for the Safety Assessment SR-Site	Section 2.3, 3.2	
TR-10-13, Spent Nuclear Fuel for Disposal in the KBS-3 Repository	Sections 1, 2, 6, Appendices A - D	
TR-10-50, Radionuclide Transport Report for the Safety Assessment SR-Site	Section 3, Appendices E & F	

TR-10-61, Simple Functions Spreadsheet Tool Presentation	Sections 1, 2 (part), 3.1.1, 5-6, Appendices A & B
R-10-50, Determination and Assessment of the Concentration Limits to be used in SR-Can. Supplement to TR-06-32	Tables 2-2 to 2-4
TR-06-32, Determination and Assessment of the Concentration Limits to be used in SR-Can	Section 3, Table 5-1, 8-1, Appendix C (part)
TR-06-17, Update of a Thermodynamic Database for Radionuclides to Assist Solubility Limits Calculation for Performance Assessment	All sections at a high level
TR-10-51, Model Summary Report for the Safety Assessment SR-Site	Section 3.20
TR-10-66, Corrosion Calculations Report for the Safety Assessment SR-Site	Section 4.3.4, Appendix 1
R-09-04, Strategy for Thermal Dimensioning of the Final Repository for Spent Nuclear Fuel	Section 3.3.3, Appendix C
TR-09-22, Design Premises Report	Brief skim Section 2.4
TR-10-15, Design, Production and Initial State of the Buffer	Section 3.1.3, 4.2, 6.1.1
R-06-73, Deep Repository – Engineered Barrier Systems. Geotechnical Properties of Candidate Backfill Materials – Laboratory Tests and Calculations for Determining Performance	Section 1
TR-10-47, Buffer, Backfill and Closure Process Report for the Safety Assessment SR-Site	Section 2, 3 (part), 4 (part)
R-09-20, Groundwater Flow Modelling of Periods with Temperate Climate Conditions – Forsmark	Section 6 (part)

APPENDIX 2

Suggested Needs for Complementary Information from SKB

The list below records suggested questions to SKB for clarification and complementary information as identified during this review.

1. It is stated in Section 2.3 of the "SDK-003 Quality Assurance Plan for the Safety Assessment SR-Site" (SKBdoc 1064228, version 3.0) that an internal QA audit was ordered by the SR-Site project to be held during the first half of 2009. Did this audit take place, what were the findings and were there any non-conformities to be addressed?
2. The SR-Site Data Report only includes data identified by SKB to be of particular significance for assessing repository safety. However, whilst it is stated that data are identified through analysis of the Assessment Model Flowcharts and the radionuclide transport assessment, there is no discussion of the decision criteria. What are the criteria used to determine if data are "essential" and therefore should be in Data Report?
3. It should be clarified whether data not included in the Data Report, whether regarded as essential or not, are subject to any QA requirements other than those covered by general review of the report in which it is presented. As defined in the SR-Site QA steering documents, only data regarded as essential and presented in the Data Report appear to be covered by specific data QA requirements. If data are presented in reports other than the data report, are they still qualified to the same standard and checked? What procedure is used?
4. SKB maintains a centralised model storage area where models, source codes and other kinds of files, such as Excel spreadsheets, are stored (Section 1, "Instruction for Model and Data Quality Assurance for the SR-Site Project", SKBdoc 1082128, Version 1.0). However, SKB does not require codes used and owned by contractors to be stored in the model storage area. In this case, how does SKB ensure that it maintains access to the models used in the assessment and that SKB is not overly dependent on a single contractor for models? Further, does SKB independently audit the models and assessments developed by contractors?
5. The latest version of the QA instruction "Supplying Data for the SR-Site Data Report " (SKBdoc 1082129, version 4.0) is dated 5 May 2011 yet the SR-Site Data Report was published in December 2010 and the Main SR-Site Report in March 2011. The comments in the procedure revision history note that the responsibility for data qualification approval has been redefined and that a number of demands on the supplier and/or customer have been softened to reflect Section 2.3 in the Data Report. This indicates that the supply of data to the Data Report did not follow the requirements set out in the QA procedure

and that the procedure was altered subsequently to reflect what did take place; why was this revision necessary? What aspect of the procedures could not be met? Which data sets were produced to the original, more stringent, procedure and which to the revised procedure?

6. Hökmark et al. (2009, R-09-04, §3.3.3) observes that: "One question, which will not be further addressed here, would be how the finish of the canister surface will change over time. If the surface finish tends to be more like 'oxidized' (e = 0.6 /CRC 1973/) or 'new' (e = 0.63 /Ageskog and Jansson 1999/) rather than between 'polished' (e = 0.023 /Cheremissinoff 1986/) and 'calorized' (e = 0.26 /CRC 1973/), after some years of exposure to the conditions in the deposition hole, this would increase the effective conductivity and reduce the temperature gap". Is this question addressed in SR-Site, and if so, where?

APPENDIX 3

Suggested Review Topics for SSM

The list below records recommendations for issues requiring more detailed review in the SSM Main Review Phase.

1. This initial review has focused on the traceability of data presented in the SR-Site Data Report. It is recommended that the traceability and accuracy of other parameters in the Data Report not considered here are reviewed in the Main Review Phase, particularly parameters from the Surface System Data chapter, which has not been considered. Further, it is recommended that parameters qualified in reports other than the Data Report are reviewed, especially as it is not clear that such data are subject to any specific data QA procedure.
2. It is recommended that, considering the significance of solubility in the radionuclide transport calculations, that solubility data are investigated in more detail in the Main Review Phase. The traceability of the solubility data presented in the SR-Site Data Report (Section 3.4) is poor. An outstanding activity from this review is to check the recommended data against Hummel *et al.* (2002), the Nagra/PSI chemical thermodynamic database (see Section 4.1.2 in this report for further detail). Further, the transfer of the recommended equilibrium constant values from the Data Report into the Simple Functions spreadsheet should be reviewed and the transfer of the calculated solubility limits into the COMP23 radionuclide transport modelling. This review will require access to SKB's model input and output files. The Radionuclide Transport Report (§3.7.3) cites two unpublished documents that may contain a record of the solubility limit calculations and should be considered in the Main Review Phase:
    - SKBdoc 1260107 version 1.0 "Supporting calculations related to radionuclide tramsport[sic]", SKB, 2010.
    - SKBdoc 1260297 version 1.0 "Scripts and input data used for radionuclide transport calculations with COMP23", SKB, 2010.

   The Model Summary Report (SKB, 2010b, §3.20.5) also cites (SKBdoc 1265616, Table 1-2) for data used in SR-Site that are archived at SKB, which may prove relevant.
3. Flow-path data are not presented in the Data Report but unpublished SKB documents that are said to contain the equivalent flow rate, advective travel time and flow-related transport resistance data that are used in the models are cited (SKBdoc 1255039 and SKBdoc 1256019). It is recommended that SSM requests these documents from SKB and reviews the data, their traceability and their application in the hydrogeological modelling.

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

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

The Authority reports to the Ministry of the Environment and has around 270 employees with competencies in the fields of engineering, natural and behavioural sciences, law, economics and communications. We have received quality, environmental and working environment certification.

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