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Supplying data for the SR-Site Data Report

APPENDIX 5 to SDK-003 Quality assurance plan for the safety assessment SR-Site (Document ID 1064228)

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1 Introduction

1.1 Purpose of the instruction

This document is an instruction issued by SKB that should be followed by suppliers and customers of data in the process of developing the SR-Site Data report. This instruction should be read as a supplement to the quality assurance document [SDK-003 Quality assurance plan for the safety assessment SR-Site \(Document ID 1064228\)](#).

1.2 Scope of the instruction

This instruction should apply to all suppliers of data to the Data report and to the customer (the SR-Site team). It should apply to all data of all subject areas of the Data report. A list of all data compiled in the Data report will be given in the Data report. The Data report concerns data that are identified to be of particular significance for the SR-Site safety assessment.

There are several issues related to data that are not covered by the Data report. Evaluation of processes and selection of models fit for use in the assessment process will be made in different Process reports. Selection of scenarios and calculation cases, which in turn define the conditions for which data need to be supplied, will be made in the SR-Site Main report. The initial state of the system is given in a series of Production reports. Descriptions of the sites will be given in the Site descriptive model reports.

1.3 Background to instruction and need for data qualification

The objective of the Data report is to compile input data, with uncertainty estimates, for the SR-Site assessment calculations for a wide selection of conditions. Data should be assessed through standardised procedures, adapted to the importance of the data, aiming at identifying the origins of uncertainties and in which the input provided by suppliers is distinguished from judgements made by the assessment team.

All input data used in quantitative aspects of the safety assessment have uncertainties associated with them. The quality of the results of any calculation in the assessment will, among other factors, depend on the quality of the input data and on the rigour with which input data uncertainties have been handled. A methodological approach for the qualification of input data with uncertainties and the subsequent handling of data uncertainty is therefore required.

In SR 97, a standardised procedure was employed for all input data to radionuclide transport calculations. These data were presented in the SR 97 Data report /Andersson, 1999/ which was jointly reviewed by the authorities as part of the SR 97 review /SKI/SSI, 2001/. Following SR 97, both SKB /Hedin, 2002; Hedin, 2003/ and the authorities /Wilmot and Galson, 2000; Wilmot et al., 2000; Hora, 2002; Hora and Jensen, 2002/ have performed investigations relevant to the data derivation process in safety assessment calculations. Among other things, the reviewers of the SR 97 assessment required quantification of uncertainties into a form suitable for probabilistic assessment and traceable records on the expert input to data selection and uncertainty assessment.

The results of these studies and the general development, work undertaken were initially reported and applied in the interim version of the SR-Can Data report /SKB, 2004/ which was developed to show how the safety assessment methodology has been developed since SR 97. The Interim version of SR-Can was followed by the SR-Can assessment and the SR-Can Data report /SKB, 2006/ in which site specific data were (naturally) to a much larger extent included. Also the SR-Can Data report /SKB, 2006/ was reviewed by the authorities /Dverstorp and Strömberg, 2008/. The general conclusion of that review was that the structure of the Data report and the templates provides the basis for providing the data necessary for the analysis. However, the authorities also concluded that there were no clear distinction between data that were included in the Data report and data that were reported elsewhere. Neither was there a clear enough distinction between opinions given by the experts supplying data and by the SR-Can team.

Moreover, the authorities identified cases where the data selection process was not transparent and also traceability issues on how data were used later on in the assessment.

This instruction has been written to facilitate methodical and traceable data qualification, where comments made by authorities form a basis for the improvements in the data qualification methodology.

1.4 Application of the instruction

1.4.1 Parts concerned by the instruction

This instruction concerns three parts, the suppliers, the customer, and the Data report team responsible for approving the data and data qualification procedure. The Data report is divided into different subject areas, and for each subject area a supplier and a customer are identified.

The suppliers supply data to the Data report. The suppliers are the teams originating or compiling the data, as described in the site-descriptive model reports, production reports, and other supporting documents. The author producing text for the Data report on behalf of the supplier is called the supplier representative. The supplier representatives should represent the teams, and not rely solely upon their own opinions.

The customer is in broader terms the SR-Site team that is responsible for performing the SR-Site safety assessment. However, the entire team is not generally involved in each subject area but it is rather embodied by a group of persons with special knowledge and responsibility. The author producing text for the Data report on behalf of the SR-Site team is called the customer representative. The customer representatives should represent the SR-Site team, and not rely solely upon their own opinions.

The Data report team is a subgroup to the SR-Site team. The Data report team has written this instruction, administrate the Data report, and write the general text in the Data report that does not concern specific data. The Data report team has also an editorial role of the subject area sections. The appropriate Data report team member is responsible for reporting the procedure with which the data were qualified. This is done by writing the protocol(s) from the data qualifications meetings. The protocol(s) is finally approved by the project leader of the SR-Site project. Thereafter the data are formally considered as qualified.

The persons being supplier representatives, customer representatives, and members of the Data report team will be listed in the protocol of the data qualification meetings, and in the SR-Site expert list.

1.4.2 The initiation of a subject area

Upon identification of the supplier or customer representatives, and after they accept their tasks, this instruction is presented. This is generally done during a meeting between the supplier and/or customer representative and a member of the Data report team. It is agreed that the text supplied to the Data report should be written according to the instruction, to the extent possible. In case of further questions or unresolved issues, the supplier and/or customer representatives should contact the Data report team.

1.4.3 The writing of a subject area

The supplier and/or customer representative is given a Microsoft Word template for the Data report. Text should only be written in the subject area section assigned to the supplier and customer representatives, even though other sections can be viewed.

The customer representative should write subsections x.x.1 and x.x.2 (see Chapter 2 of this instruction for explanation) defining what data should be delivered by the supplier, and putting the data into a context of safety assessment modelling. Based on this text, the supplier representative should write subsections x.x.3 to x.x.10, discussing sources of information, various variability and uncertainty, and delivering the requested data (see Chapter 2). Thereafter, the customer representative writes subsections x.x.11 and x.x.12, where a judgement is made and data are finally selected for use in SR-Site. Throughout the writing of the text, the Data report team provides support.

1.4.4 Data qualification meeting

When the entire text is written, a data qualification meeting is held. On this meeting the customer and supplier representative, together with at least one member of the Data report team should attend. Others may also attend. At the meeting, a checklist is gone through; with the purpose of controlling that the procedures of performing and documenting the data qualification have been followed. This results in one of the following two cases:

- If there are no deviations and no actions are required, a protocol from the meeting including the checklist is established and stored in SKBdoc. The version of the approved document is recorded in the protocol.
- If there are deviation and actions are required, these are listed in an action list associated with the checklist. Upon completions of each action, a comment is written in the action list. When all actions are completed, the modified text is distributed to all parts. Upon approval from all parts, a protocol from the qualification meeting including the checklist and also the action list and comment on handling the actions is established and stored in SKBdoc. The version of the approved document is recorded in the protocol.

It is sufficient to store one combined protocol from the data qualification meetings in SKBdoc, as long as it includes check lists and notes from all meetings held. This protocol should be finally approved by the project leader of the SR-Site project.

1.4.5 Control of data when finalising the Data report

After the Data report has been reviewed and is finalised, it is controlled by the Data report team that the final data are identical to the data approved upon on the data qualification meeting. If not, the reasons for the deviation are investigated. If the deviation results from an error, the error is corrected. If the deviation results from an active decision, the deviation is brought to the attention of the SR-Site team. A general forum for this is the SR-Site project meetings, but to the extent possible individual users of the data should be alerted as soon as possible.

It is reminded that the users of the data should take actions to check that preliminary data used in calculations and modelling coincide with the final data. However, such a check is regulated by the quality assurance document [Appendix 7 to SDK-003, Final control of data used in SR-Site calculations/modelling \(Document ID 1186612\)](#).

2 Qualification of input data – instruction to supplier and customer

The final objective of the Data report is at performing data qualification including estimates of both conceptual and data uncertainty, as well as of natural variability, for various subject areas. In addition, the traceability of the data is examined. The qualified data are intended for use as input data in the SR-Site safety assessment modelling.

The Data report does not concern all data used in the SR-Site safety assessment, but those which are identified to be of particular significance for assessing repository safety. Data may concern both measured data from the laboratory and from the field, as well as output from detailed modelling where measured data are interpreted, depending on the subject area. Even though the data may represent both parameters and entities, in this instruction the word “data” is generally used.

It should be pointed out that in the process of qualifying data, the traceability that is the focus of many quality assurance systems is only one aspect. An equally important aspect is the scrutinising of the scientific adequacy of the data.

Each set of data provided in the Data report is categorised into one of many different subject areas. For each subject area, the data qualification process comprises a sequence of stages resulting in a text of a standard outline. The sequence of stages and the standard outline are shown in Figure 1.

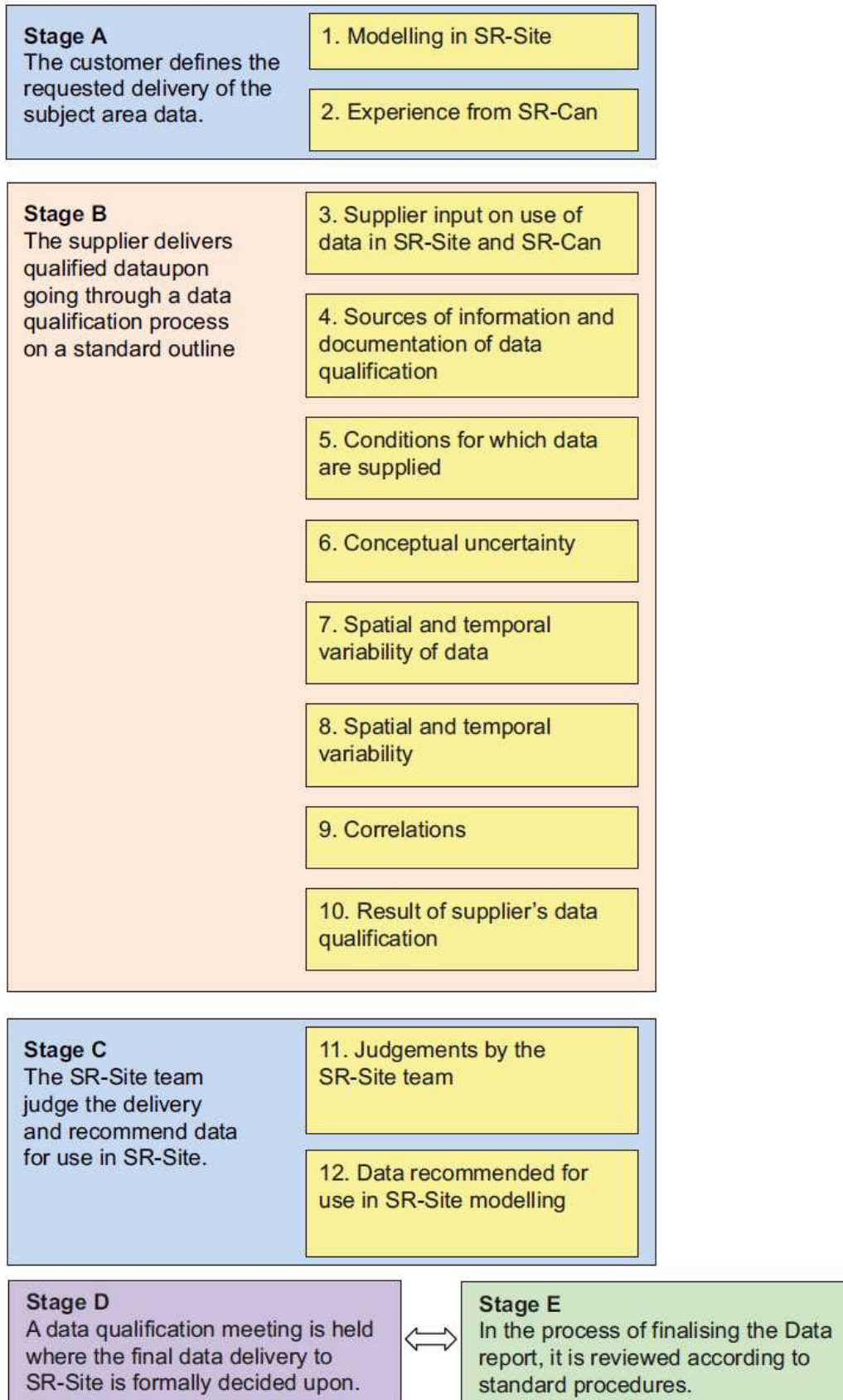


Figure 1. Stages of writing and reviewing the Data report. The standard outline of a subject area is shown in the yellow boxes.

Below, the parties involved in the Data report and the sequence of stages shown in Figure 1 are discussed. The standard outline is described in Sections 2.1 to 2.12.

For each subject area, the Data report team identifies the customer and supplier of data, and assigns a customer representative and a supplier representative that co-author the subject area section¹.

The customer is in broader terms the SR-Site team that is responsible for performing the SR-Site safety assessment. However, the entire team is generally not involved in each subject area but it is rather embodied by a group of persons with special knowledge and responsibility. The customer representative should represent the SR-Site team, and not rely solely upon own opinions.

The suppliers are the teams originating the sources of data, for example the site descriptive model reports, production line reports, and other supporting documents. The supplier representative should represent the team, and not rely solely upon own opinions.

The intended chronology of the writing of a subject area section is the following.

- Stage A: The customer representative writes the first two sections defining what data are requested from the supplier, how the data will be used in SR-Site modelling, and how similar data were used SR-Can modelling.
- Stage B: The supplier representative writes the following eight sections that are the core of the data qualification. This is done according to a standard outline where a number of issues such as traceability, data uncertainty, and natural variability should be dealt with. These sections should result in sets of qualified data that are the delivery to the customer.
- Stage C: The customer representative, representing the entire SR-Site team, writes the last two sections making judgements upon the delivery and recommending data for use in SR-Site modelling. The text is produced in close cooperation with other persons within the SR-Site team with special knowledge and responsibility. The text should reflect upon the formal decision taken in Stage D (accordingly, it may need to be revised after Stage D).

The text of each stage should be made available in good time to the person or persons responsible for writing the text of the subsequent stage. Upon completion of Stage C, a data qualification meeting is held (Stage D) and the text is subjected to factual review (Stage E). If case the subject area text has been well communicated during its preparation, and the customer and supplier share the views of the text, the data qualification meeting (Stage D) may be held after the factual review (Stage E), to get an external input on the data delivered.

- Stage D: For each subject area, a data qualification meeting is held where the customer and supplier representatives, and at least one member of the Data report team are invited. Appropriate members of the SR-Site team and supplier team may also be are invited. At the meeting, the data delivery to SR-Site is formally decided upon and the decision is recorded in minutes (documented according to SKB's quality assurance system).
- Stage E: The subject area section is subjected to factual review according to standard procedures.

Finally, within the SR-Site project but outside the scope of the Data report team, a follow-up is made where it is controlled that the correct data are used in SR-Site modelling. This could be seen as Stage F in the data qualification process, but its falls upon the modellers using the data to carry this stage through. It is therefore not shown in Figure 1.

In the following sections, the outline shown in the yellow boxes in Figure 1 is described in detail.

¹ The terms customer and supplier come from standard quality assurance terminology.

2.1 Modelling in SR-Site

In this section, the customer representative should define what data are requested from the supplier, and give a brief explanation of how the data of the subject area are intended to be used in SR-Site modelling activities.

2.1.1 Instructions to the customer representative

The customer representative should start by carefully defining what data are requested from the supplier. Thereafter, the modelling activities that data are used in should be shortly described.

Defining the data requested from the supplier

Here, the customer should define the data (parameters) that should be part of the supplier's delivery, in a bullet list. If applicable, the parameter symbol and unit should be provided in this list. If the supplier should focus on providing data of certain ranges, or for certain conditions, this should be specified. This text should not only facilitate the task of the supplier, but also assist the reader of the Data report in understanding the scope of the subject area section.

SR-Site modelling activities in which data will be used

Here the customer should give a brief explanation of how the data are intended to be used in different SR-Site modelling activities. This explanation should cover both how the data are used in specific models, and in the SR-Site model chain (unless evident from the assessment model flowcharts). Differences from the use of this type of data in SR-Can should be highlighted. The justification for the use of these models in the assessment is provided in other SR-Site documents, such as the SR-Site Main report and process reports.

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 the model chain may be modified. As a result, this text 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.

2.2 Experience from SR-Can

In this section the customer should give a brief summary on how the data of the subject area were used in SR-Can. The experience from SR-Can should function as one of the bases for defining the input data required in SR-Site modelling. It should be noted that the teams undertaking the SR-Site and SR-Can safety assessments largely are the same, so transferring experience from SR-Can to SR-Site should not present any substantial problem.

2.2.1 Instructions given to the customer representative

The summary of how the data were used in SR-Can should conform to the following outline:

- Modelling in SR-Can.
- Conditions for which data were used in SR-Can.
- Sensitivity to assessment results in SR-Can.
- Alternative modelling in SR-Can.
- Correlations used in SR-Can modelling.
- Identified limitations of the data used in SR-Can modelling.

More detailed guidance regarding what should be included in the summary in relation to each of these bullets is given below.

Modelling in SR-Can

The use of the data in specific SR-Can models, as well as in the SR-Can model chain, should be described. As such an account is generally included in the SR-Can Data report /TR-06-25/, the summary

should be kept short and focus upon differences between the use of data in SR-Can and SR-Site. Repetitions from the section “Modelling in SR-Site” should be avoided. If there is no difference between the SR-Can and SR-Site modelling approaches, it is sufficient to state this.

Conditions for which data were used in SR-Can

In this subsection, the relevant conditions to which the subject area data were subjected to in SR-Can modelling should be outlined. Relevant conditions are only those conditions that significantly influence the data, in the context of demonstrating repository safety. Different subject area data are affected by different conditions. For example, the sorption partition coefficient K_d may be strongly influenced by groundwater salinity. Thus, in characterising the conditions under which K_d values were used, it is likely to be appropriate to give the salinity range during repository evolution, for example as assessed in the SR-Can hydrogeochemical modelling. Other types of conditions may include gradients, boundary conditions, initial states, engineering circumstances, etc.

It is sufficient to state the relevant conditions used in SR-Can modelling (including those applied in sensitivity analyses, various initial states, different scenarios, and evolution within scenarios) and to refer to SR-Can documents for background information. Justification as to why those conditions were studied is not required. Where appropriate, the relevant conditions should be tabulated. It should be noted that the stated conditions do not restrict qualification of data for use under other conditions, but merely underline the conditions considered appropriate within the modelling context of SR-Can. If conditions of SR-Can were similar to those of SR-Site, it is sufficient to state this.

Sensitivity to assessment results in SR-Can

In answering the above, the customer representative should consider if the cited sensitivity analyses were sufficiently general to provide definitive answers.

Where appropriate, an account should be given of results from sensitivity analyses performed as part of, or prior to, the SR-Can safety assessment. Such analyses were made in order to prioritise uncertainty assessments for those data and conditions judged to be potentially important for performance, both for overall end-points such as risk and for conditions affecting the state of the system. If such sensitivity analysis was performed, the following issues may be outlined:

- For what ranges of the data was the impact on the SR-Can safety assessment significant and are there ranges where the impact was negligible? If sensitivity analyses show that only part of the range has an impact on repository safety, less effort may be given to quantifying parameter values outside this range.
- Was the impact monotonic, i.e. is there a unidirectional relationship between the data value and performance, is there an “optimal” value, or is the impact dependent in a complicated manner upon the values of other input data?
- What degree of variation in the data is needed to have an impact on safety assessment results (this may be different for different data ranges)?
- Were the results applicable to all conditions of interest – or only to some?

In discussing the above, the customer should consider if the cited sensitivity analyses were sufficiently general to provide definitive answers.

Alternative modelling in SR-Can

Whenever it applies, the customer should summarise alternative modelling in SR-Can focusing on the concerned data. The following issues should be reflected upon:

- What alternative models exist and what influence did they have on the safety assessment?
- Were conceptual uncertainties, related to the models in which the data were used, identified in SR-Can? In that case, what was the impact on assessment results?

Correlations used in SR-Can modelling

A correct treatment of probabilistic input data requires that any correlations between those data are identified and quantified. The correlations associated with the subject area data, as accounted for in SR-Can, should be briefly described. This includes internal correlations within the subject area and correlations with data of other subject area sections. If the same correlations were used as will be used in SR-Site, it is sufficient to state this.

Identified limitations of the data used in SR-Can

If limitations or shortcomings of the data used in SR-Can have been identified, which may significantly have affected the assessment, such should be accounted for. The limitations or shortcomings can be due to, for example, lack of site-specific data or lack of data obtained at conditions representative for the repository. The limitations and shortcomings may have been identified by the regulatory authorities, by SKB, or by other parties.

2.3 Supplier input on use of data in SR-Site and SR-Can

2.3.1 Instructions to the supplier representative

In this section the supplier has the opportunity to comment on the two above sections. The focus for the supplier should be to help the SR-Site team in choosing appropriate data and modelling approaches, and avoid repeating errors and propagating misconceptions from SR-Can or from earlier safety analyses. Even if a single individual has the roles as both supplier and customer representative, he or she may still make comment upon the use of data in SR-Site and SR-Can.

2.4 Sources of information and documentation of data qualification

This section is devoted to presenting the most important sources of data, as well as categorising different data sets on the basis of their traceability and transparency, and scientific adequacy. Sources of data may include SKB reports, SKB databases, and public domain material. Documents of importance for the data qualification may also consist of SKB internal documents. All underlying documents should be properly cited throughout the Data report.

2.4.1 Instructions to the supplier representative

Sources of information

The supplier is asked to tabulate the most prominent references used as sources of data. In addition, the references of important documents describing the process of acquiring, interpreting, and refining data may be listed.

If the data qualification process is well documented in supporting documents, it is sufficient to reference these documents and to only briefly summarise the data qualification process. If not, the Data report gives the supplier a chance to appropriately document the data qualification process of the subject area data.

Concerning sources of information, the supplier should:

- Fully cite all sources of information throughout the text. It is necessary to keep in mind that the text may have readers with limited in-depth knowledge of the subject. Therefore, what normally would seem as trivial may deserve references for further reading. It is strongly recommended to make an extra effort to refer to the open literature where possible, and not only to SKB documents.
- In case of referring to a document of many pages, for example a site-descriptive model report, give detailed information on the section, figure, table, etc. where the relevant information can be found.
- Properly cite databases, SKB internal documents, etc. even though they may not be available to the general reader. In the case of referring to databases, the precise reference should be given to the individual data set used. For example, it is not sufficient to refer to the SKB database Sicada if not

also giving detailed information, such as the activity or the number of a Sicada delivery note. This is to ensure traceability within the SR-Site project.

- Fully cite advanced modelling tools where the underlying code may have implications for data qualification.

Categorising data sets as qualified or supporting

The supplier should categorise data as either qualified data or supporting data. Qualified data has been produced within, and/or in accordance with, the current framework of data qualification, whereas supporting data has been produced outside, and/or in divergence with, this framework. Data taken from peer-reviewed literature take a special position in that they may be considered as qualified even though they are produced outside the SKB framework of data qualification. However, such data are not by necessity categorised as qualified, as they may be non-representative or lack in some other aspect.

Data recently produced by SKB, for example in the site investigations, should a priori be considered as qualified. However, before the data are formally categorised as qualified, a number of considerations need to be made as described below. Data produced outside the data qualification framework should a priori be considered as supporting data. This could for example be data produced by SKB prior to the implementation of its quality assurance system, or data produced by other organisations. Before formally categorise the data as supporting, a number of considerations need to be made as described below.

Data taken from widespread textbooks, engineering handbooks, etc., which are considered to be established facts, need not to be scrutinised. Well-known data that should be excluded from the Data report need not to be categorised as qualified or supporting data, although their exclusion may need to be justified.

It is outside the scope of the Data report to deal with individual data. Instead the supplier should characterise data sets as qualified or supporting. The supplier should decide to what extent various data can be included in a single data set for the specific case. The following examples of natural barrier data sets could be used for inspiration:

- Data, or part of data, obtained by a specific method at a site, rock volume, borehole, etc.
- Data, or part of data, obtained by various methods at certain conditions (e.g. saline water) at a site, rock volume, borehole, etc.
- Data, or part of data, taken from an external publication.

Qualified data

The following considerations should be made for data that a priori are identified as qualified, before formally categorising them as qualified. Most of the data that is delivered to the Data report are refinements and interpretations of observed data. Such refinements and interpretations are performed both for engineered and natural barrier data. For example, the multitude of data acquired within the site investigation are normally refined within the site-descriptive modelling by use of more or less complex models. The supplier should judge whether data acquisition and refinement, and associated documentation, are in accordance with the implemented data qualification framework. The following considerations may form the basis for the judgement.

Considerations concerning data acquisition:

- Is the acquisition of observed data performed in conformance with a widely adopted quality management system (e.g. the ISO 9000 series or equivalent)?
- Is it possible to trace relevant quality assurance documents (for example method descriptions, field notes, etc.) for the measurements? It should be noted that even though the quality assurance documents may not be available for the general reader, they are accessible for the SR-Site team.

- Is it possible to extract relevant information on the data quality, variability, and representativity from documents reporting the acquisition of data?
- Are concerns associated with the observed data and nonconformities of the measurements transparently described?
- Is the undertaken data acquisition programme sufficient to determine the full range of data uncertainty and natural variability, and do the acquired data appropriately characterise the intended aspect of the system (site, rock domain, copper canister, population, etc.)?

Considerations concerning data refinement:

- Are concerns and nonconformities described in the supporting documents propagated to, and addressed in, the data refinement?
- In refining observed data by use of more or less complex modelling, is this done in accordance with documented methods?
- In case of more complex modelling, which may have implication for data qualification, is the details of the modelling described in either a task description or the document reporting the modelling results? Furthermore, is the modelling tool developed in accordance with a widespread quality assurance system and/or is its quality tested in other ways?
- Has comparative/alternative modelling been performed to evaluate artefacts induced in the modelling, and to evaluate whether the modelled interpretation of the data is reasonable?

Going through these questions in detail for each data set may be a too extensive task. Accordingly, the sorting of data to some degree is based on expert judgement. However, in making this judgment, it may be helpful to revisit the above bullet lists.

If appropriate data qualification has been performed and documented in supporting documents, or can be performed and documented as part of the delivery, the data should be formally categorised as qualified data. If the documentation of the data qualification process is inadequate in supporting documents, and appropriate data qualification cannot be performed as part of the delivery, the data must be demoted to the category supporting data.

As mentioned before, data taken from peer-reviewed literature takes a special position in that they may be considered as qualified even though they are produced outside the SKB framework of data qualification. However, before formally categorising them, one needs to judge whether they are representative for the intended KBS-3 repository system and the Forsmark site. A prerequisite for making such a judgement is often that the documents are transparently written. In case the data are non-representative for Swedish conditions, or their degree of representativity is difficult to evaluate, the data may be categorised as supporting instead of as qualified.

Supporting data

The following considerations should be made for data that a priori are identified as supporting, before formally categorising them as supporting. Such data are produced by SKB outside the framework of data qualification, or by other organisations. The supplier should:

- Consider how well the method used to acquire the data is described? The greater the transparency with which the method is described in the supporting document, the greater the value should be ascribed to the data.
- Consider how well the method used to interpret and refining the data is described? The more transparently the interpretation and refinement is described in the supporting document, the greater the value should be ascribed to the data.

- Consider if it is possible to identify and evaluate the data qualification process used in acquiring and refining the data? If it is shown that a sound data qualification process has been used, the data should be ascribed greater value.
- Judge, based on the above, whether the data can be used as part of the basis for recommending data to SR-Site safety assessment modelling, as comparative data for other qualified data, or should not be used at all. In some cases the transparency of a document is so poor that crucial information concerning data qualification cannot be extracted. If this renders an assessment of the data's scientific adequacy and their representativity for Swedish conditions impossible, the supplier should recommend that the data are dismissed. This can be done even if the numerical values of the data are consistent with other, qualified data.

In case data that a priori are assumed to be supporting are acquired, interpreted, and refined according to a similar data qualification framework as implemented by SKB, and the data are accurate and representative, the supplier can promote the data to the category qualified data.

It should be noted that data taken from peer-review literature can be categorised as supporting data. This can be done if, for example, data are only partially representative for the Swedish repository concept and the Forsmark site.

Upon formally categorising the data sets as qualified or supporting, they should be tabulated as exemplified in Table 1. As can be noted, justifications for the sorting are given in the same table for the numbered items.

Table 1. Qualified and supporting data sets (for parameter Y).

Qualified data sets	Supporting data sets
1. /SKB, 20xx/, Section 4.5: All data on parameter Y obtained for rock domain RFM029.	5. /Nilsson, 19xx/, Table 1. Data obtained in the pH range 6–9 in sedimentary rock.
2. Data presented in the Underground construction opening report in Figure x.	
3. /Svensson, 20xx/, Table 2: Data between the borehole length 400–452 m in KFM01D, indicating an average value of 2,650 m ³ /kg.	
4. All parameter Y data stored in SKB Database X, with the identity number xxx-yyy-zzz.	
1–2, 4: These data have been produced within the site investigation (item 1), within a production report (item 2), or as part of the site-descriptive modelling (item 4). These data are produced within the SKB data qualification framework and are judged as qualified.	
3: /Svensson, 20xx/ is a peer-review article and the data are obtained at the Forsmark site and are judged as representative. The data set is judged as qualified.	
5: /Nilsson, 19xx/ is a peer-review article that is transparent and scientifically sound. However, the data are predominantly representative for sedimentary rock. Accordingly they are judge as supporting.	

Excluded data previously considered as important

Within the field of nuclear waste management, there are large quantities of data that are of little significance for the SR-Site safety assessment, as they are less representative for the Forsmark site, the KBS-3 repository concept, etc. than other available data. In general, excluding such data from subsequent use in SR-Site does not require justification. The exception is if the data constitutes a well-known part of the basis of previous safety assessments (or equivalent tasks), and/or have a significant impact on the perception of the appropriate choice of data values. If it could be seen as a significant inconsistency or omission not to use the data, their exclusion should be explicitly justified. Providing an appropriate justification is particularly important if the excluded data disagree with the presently used data.

2.5 Conditions for which data are supplied

The data of the different subject areas are likely affected by different conditions. Conditions refer to initial conditions, boundary conditions, barrier states, and other circumstances, which potentially may affect the data to be estimated. In the process of qualifying data for subsequent use in safety assessment, an important part is to account for the conditions for which data were acquired, and to compare these conditions with those of interest for the safety assessment.

2.5.1 Instructions to the supplier representative

In the section “Experience from SR-Can” it is stated for what conditions data were used in SR-Can. These conditions should not limit the conditions for which data are examined, but merely point out conditions that are likely to be of importance for a safety assessment. The supplier may have been given instructions from the SR-Site team, or may have opinions about important conditions, which lead to modifications of the SR-Can conditions.

In this section, the conditions for which the data have been obtained should be discussed and, as appropriate, justified as relevant to SR-Site. Such a condition is often a single value (e.g. temperature), a range (e.g. salinity range), or a gradient (e.g. hydraulic gradient). Other factors of relevance for repository safety may be included as conditions, at the discretion of the supplier. Conditions that are deemed to be of particular importance for repository safety should be highlighted. Other conditions that do not significantly relate to repository safety, but may be of importance for data qualification, are also important to note. Such information is valuable when, for example, crosschecking data sets with those of other studies or evaluations. The supplier may list ranges of applied conditions during data acquisition, excluding conditions that are both general and self-evident (such as the gravitation).

In many cases, it is expected that the conditions for which data are supplied will differ from those assumed in the SR-Site safety assessment. For example, a set of supplied data may not represent the full temperature range required, or may have been obtained at a different pressure than expected in situ. The differences identified by the supplier should be outlined in this section. Furthermore, for each deviating condition of importance for the assessment results, the implications should be discussed.

2.6 Conceptual uncertainty

This section concerns conceptual uncertainty of the subject area data. Two types of conceptual uncertainty should be discussed. The first concerns how well the data, and the models wherein they are used, represent the physical reality, and the second concerns conceptual uncertainties introduced in the acquisition, interpretation, and refinement of the data.

2.6.1 Instructions to the supplier representative

In this subsection, the supplier representative is required to reflect on the conceptual uncertainty of the subject area data. Generally data are included in models that represent an idealised reality, which to some degree differs from the physical reality. Therefore, one can expect that a degree of conceptual uncertainty is associated with all data compiled in the Data report.

To the extent possible, the supplier should describe such conceptual uncertainty. This should be done in the context of the models in which the data are used, intended to describe certain postulated processes. Also, it may be appropriate to discuss alternative conceptualisations in which the data may be used in different ways. If comprehensive discussions on the subject have already been documented, such documents may be referred to and a short summary of the conceptual uncertainty will suffice. Aspects of the conceptual uncertainty that are obviously unrelated to repository safety may be disregarded.

Conceptual uncertainty may also be introduced in the acquisition, interpretation, and refinement of the data. For example the data may have been obtained by inverse modelling of experimental results, where conceptual uncertainty is introduced by the model. The data may also have been obtained by using some correlation relationship, where there is conceptual uncertainty in the correlation. Many other sources of

conceptual uncertainty are conceivable and may be discussed at the discretion of the supplier. In doing this, the supplier should carefully differentiate between uncertainties introduced due to conceptual issues and data uncertainty introduced by measurement errors, etc. Data uncertainty should be discussed in the following section.

2.7 Data uncertainty due to precision, bias, and representativity

In this section data uncertainty should, if possible, be discussed in terms of precision, bias, and representativity, in the context of their application in SR-Site. Such uncertainty is associated both with the acquisition of data, for example in the site investigations, and subsequent refinement of data, for example in the site-descriptive modelling. Data uncertainty includes neither conceptual uncertainty nor natural variability.

2.7.1 Instructions to the supplier representative

The supplier representative should discuss the data uncertainty in terms of precision, bias, and degree to which the data are representative in the context of their application in SR-Site. If comprehensive discussions on these matters are documented elsewhere, such documents should be referred to, and a short summary of the discussion will suffice. The supplier should begin with discussing the precision of the supplied data. To the extent possible, data spread due to the precision should be separated from data spread due to natural variability. Precision issues are both associated with the method used in acquiring the raw data and subsequent interpretation of data. Concerning acquiring raw data, limitations in precision are not only associated with the equipment and method used when performing the measurements, but also with the sampling procedure, sample preparation, etc. Precision issues associated with interpretation of the data depend to a large degree on the procedure used, and should be discussed at the discretion of the supplier. As an example, it may not be straight forward to estimate the precision of data that are a function of other acquired data, with their intrinsic limitations in precision.

Thereafter, the supplier should discuss the bias of the supplied data. Similar considerations apply as when discussing precision, both for bias associated with the acquisition of raw data and with their subsequent interpretation. Bias in observed data is often associated with the method used for acquiring data and its calibration, and with effects of sample preparation. Bias is also associated with the sampling procedure, sample size, and differences in conditions for example between those in the laboratory and in situ. Bias issues associated with data interpretation depend to a large degree on how the interpretation is made, and should be discussed at the discretion of the supplier.

Finally the supplier should discuss the representativity of the supplied data, both in terms of data acquisition, and data interpretation and refinement. Issues associated with the representativity of acquired data often concern the sampling procedure, the sample size relative to natural variability and correlation length, and differences in conditions between, for example, those in the laboratory and in situ.

An important issue is whether the data are generic or site and/or technique specific. In the case of access to generic data only, the supplier should discuss whether, and to what degree, the lack of site and/or technique specific data influences the data uncertainty. Representativity issues associated with data interpretation and refinement depend much on the specific interpretation and refinement process, and should be discussed at the discretion of the supplier.

As well known, the precision, bias, and degree of representativity often depend on a mixture of the above-suggested sources for data uncertainty, and may not be easily separated. However, the supplier is asked to reflect carefully on these issues, as an assessment of data uncertainty is central for the data qualification. In case data uncertainty cannot be discussed in terms of precision, bias, and representativity, for example as the resolution in data does not allow for such separation, it will suffice to make a general data uncertainty discussion.

Comprehensible illustrations of different data sets are of high value. The objective of the illustrations is not necessarily to provide a detailed basis and description of the numerical values of the individual data.

Sometimes the objective may be to give the reader an understanding of how much, and in what ways, the data varies and the data sets differ from each other. An example of presenting different data sets is given in Figure 2, where the reader can get an immediate perception about differences between the data sets. Examples of other illustrations are given in Section 2.10.

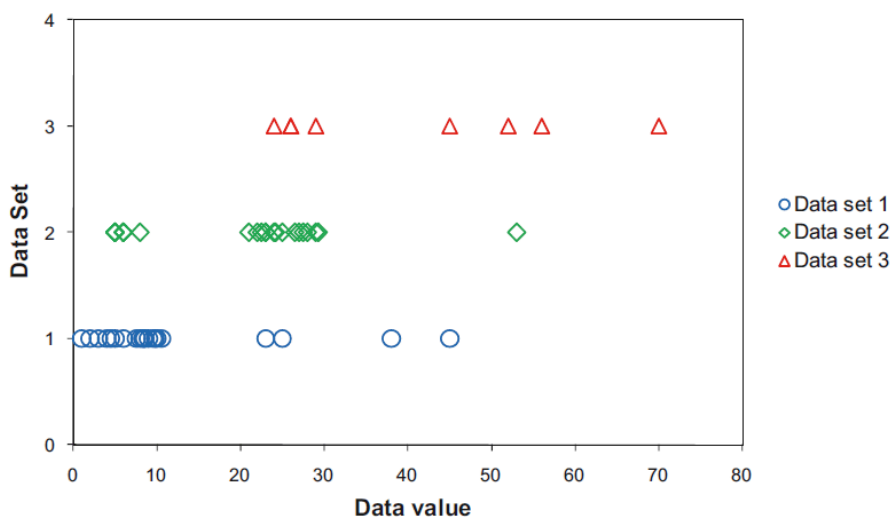


Figure 2. Example of presenting differences in data sets.

2.8 Spatial and temporal variability

In this section the supplier should discuss the spatial and temporal variability of the subject area parameters. The natural variability should as far as possible be separated from data uncertainty, discussed in the above section.

2.8.1 Instructions to the supplier representative

In this section the supplier should describe what is known about the spatial variation, sometimes referred to as heterogeneity, of the subject area data. This may result in different data sets for different volumes or elements of the repository system, or for different time periods. If comprehensive discussions on the natural variability are documented elsewhere, such documents should be referred to and a short summary of the natural variability will suffice.

- In the process of describing the spatial variability, it may be helpful to reflect on the following line of questions.
- Is there spatial variability of the data, and if so is it of consequence for the safety assessment?
- Is the spatial variability scale dependent? If so, can an appropriate approach of upscaling to safety assessment scale be recommended?
- What is known about correlation lengths from, for example, variograms?
- Can the spatial variability be represented statistically as a mean of data qualification and, if so, how is this done?
- Is there any information about the uncertainty in the spatial variability?

In the process of describing the temporal variability, it may be helpful to reflect on the following line of questions.

- Is there temporal variability of the data, and if so is it of consequence for the safety assessment?

- What processes affect the temporal variability of the data and how is the temporal variability correlated with these processes?
- Does the temporal variability follow any pattern, for example a cyclic pattern?
- Could the temporal variability be represented statistically as a mean of data qualification and if so, how is this done?
- Is there any information about the uncertainty in the temporal variability?

In addition, other relevant issues concerning the natural variability may be addressed at the discretion of the supplier. Comprehensible illustrations of different data sets from different volumes, elements, or time periods are of high value.

2.9 Correlations

An appropriate treatment of probabilistic input data requires that any correlations and functional dependencies between those data are identified and quantified. In the extensive work with the FEP database and the Process reports, most correlations and functional dependencies between parameters have been identified. Where appropriate, these correlations and functional dependencies should also be implemented in the safety assessment models. It should be an aim to aid those performing stochastic modelling, by giving well defined and usable information on how to handle correlations between input data.

Correlations and functional dependencies may also have been used when acquiring, interpreting, and refining data. For example, concerning sorption partition coefficients, data have not been acquired for all relevant radioelements. For species for which there is a lack in observations, the supplied sorption partition coefficient will have been estimated from data obtained for one of more analogue species. This has implications for how to correlate input data in stochastic safety assessment modelling.

2.9.1 Instructions to the supplier representative

In this section the supplier is requested to address the following questions:

- Are there correlations or functional dependencies between parameters within the subject area, or with parameters of other subject areas? If so, account for these and if possible also outline the consequences for subsequent modelling.
- If correlations have been used in acquiring, interpreting, and refining data, how is this done? Furthermore, is the outcome based solely upon correlations, or on both measurements and correlations?
- If the data varies in space and time – is anything known about its autocorrelation structure?
- Is there any other reason (apart from already cited correlations and functional dependencies) to suspect correlations between parameters considered as input to SR-Site modelling?

2.10 Results of supplier's data qualification

In this section the supplier is requested to present data that are considered to be appropriate as a basis for suggesting input data for use in SR-Site. Comprehensive information relating to each parameter requested in the bullet list under the heading "Defining the data requested from the supplier" (cf. Section 2.1) should be given. Only one set of data should be delivered for each specified condition, volume, element, time period, alternative modelling approach, etc.

2.10.1 Instructions to the supplier representative

The general process of reducing and interpreting data, valuing different data sets, and finally selecting the recommended data for delivery to the SR-Site team should be fully accounted for, if not already

accounted for in the previous sections or in supporting documents. In the latter case, it is sufficient to briefly summarise, or refer to, the process of selecting the delivered data.

In case the data presented in supporting documents need reinterpretation and further refinement, in the light of this instruction and/or other information, this should be fully documented. In case the supporting documents give more than one data set for a specified condition, volume, element, time period, etc., further data reduction is required. Such data reduction may include the merging of data sets, and there may be a need to give different weight to different data sets. Much weight should be given to peer-reviewed data judged as representative for the Swedish site and repository system. Generally, more weight should be given to qualified data than to supporting data. The degree to which the data are representative in the context of their application in SR-Site should also be a factor in the weighting. Exactly how much weight should be given to individual data sets must be decided upon by the supplier. The process of further reinterpretation, refinement, and data reduction should be fully documented. If it increases the readability of the text to also utilise other sections for such documentation, this is allowed. Also, if this requires much space, some information may be appended.

The data sets that the supplier recommends to the SR-Site team should be in the form of single point values, probability distributions, mean or median values with standard deviations, percentiles, ranges, or as otherwise appropriate. If the data have significant variability and/or uncertainty, the spread in data could be described as a range. However, the meaning of the range has to be provided, e.g. does it represent all possible values, all “realistically possible” values or just the more likely values? The supplier may provide more than one range, representing different probabilities, as exemplified below:

- The range wherein the likelihood of finding the data is high.
- The range for which the likelihood of finding data outside this range is very low.

All data should be recommended in the context of input data to safety assessment modelling. Accordingly the final uncertainty estimate should encompass conceptual uncertainty, data uncertainty, and natural variability (cf. Sections 2.3.6, 2.3.7, and 2.3.8). If the supplier has used some kind of mathematical expression to account for the uncertainty and natural variability, this expression should be provided and justified.

If the data are suggested to be described by a well-defined probability distribution, it should be justified on statistical grounds that the data indeed are (sufficiently well) distributed accordingly. The usage of standard deviation is often perceived to imply that the data are normally distributed; even through the definition of standard deviation is unrelated to specific probability distributions. Therefore, when giving the standard deviation, it should be remarked upon whether or not the normal distribution appropriately describes the data. If there are obvious differences between how the data set at hand is actually distributed, and the probability distribution (or range) finally recommended, the reasons for, and implications of, this should be discussed. Outliers should not be dismissed without justification.

It should be noted that in many cases, at some stage probability distributions must be assigned to numerical data being the input to probabilistic safety assessment modelling. If the supplier feels inadequate to deliver a defined distribution, but for example delivers a best estimate, an upper, and a lower limit for data, it may fall on the SR-Site team to transform such information into probability distributions. This is justified as the SR-Site team may have a better understanding of how the shape of the assigned distributions (especially in their tails) affects the assessment results. The SR-Site team may also, in some cases, have a better understanding of the underlying statistics of the suggested distribution.

The above instructions are not applicable to all data, as all data are not necessarily in the form of numerical values. Examples are exit locations for groundwater flowpaths, given as co-ordinates, or information on solubility limiting phases, given as chemical species and reactions.

For a spatially varying function well described by a given stochastic process, e.g. through a variogram or as realised in a Discrete Fracture Network, a potential statement may be that all realisations of this spatially varying function are equally probable.

Finally, it may be impossible to express the uncertainty by other means than a selection of alternative data sets. There are a number of uncertainties that cannot be managed quantitatively in any other rigorous manner, from the point of view of demonstrating compliance, than by pessimistic assumptions. This is allowed, as long as the supplier clearly documents this together with the justification for adopting this approach.

Comprehensible illustrations and tables of the suggested data sets are of high value. Figure 3 shows some examples, taken from the SR-Can Data report /SKB TR-06-25/, displaying how data may be represented. Figure 3a shows a histogram of formation factor data and also a fitted log-normal probability distribution /SKB 2006b, Figure 6-20/. The distribution parameters are displayed in the figure. Figure 3b shows an excerpt of a table displaying sorption partitioning coefficients /SKB TR-06-25, Table A-43/. Here a median value is given as the best estimate value. In addition two ranges are given, one range wherein 50% of the data are estimated to be found, and one wherein roughly 99% of the data are estimated to be found. Figure 3c, which is an excerpt of /SKB TR-06-25, Table A-6/ shows an example where no numerical data is given. Instead solubility limiting phases, used in the analysis of the solubility limits, are shown.

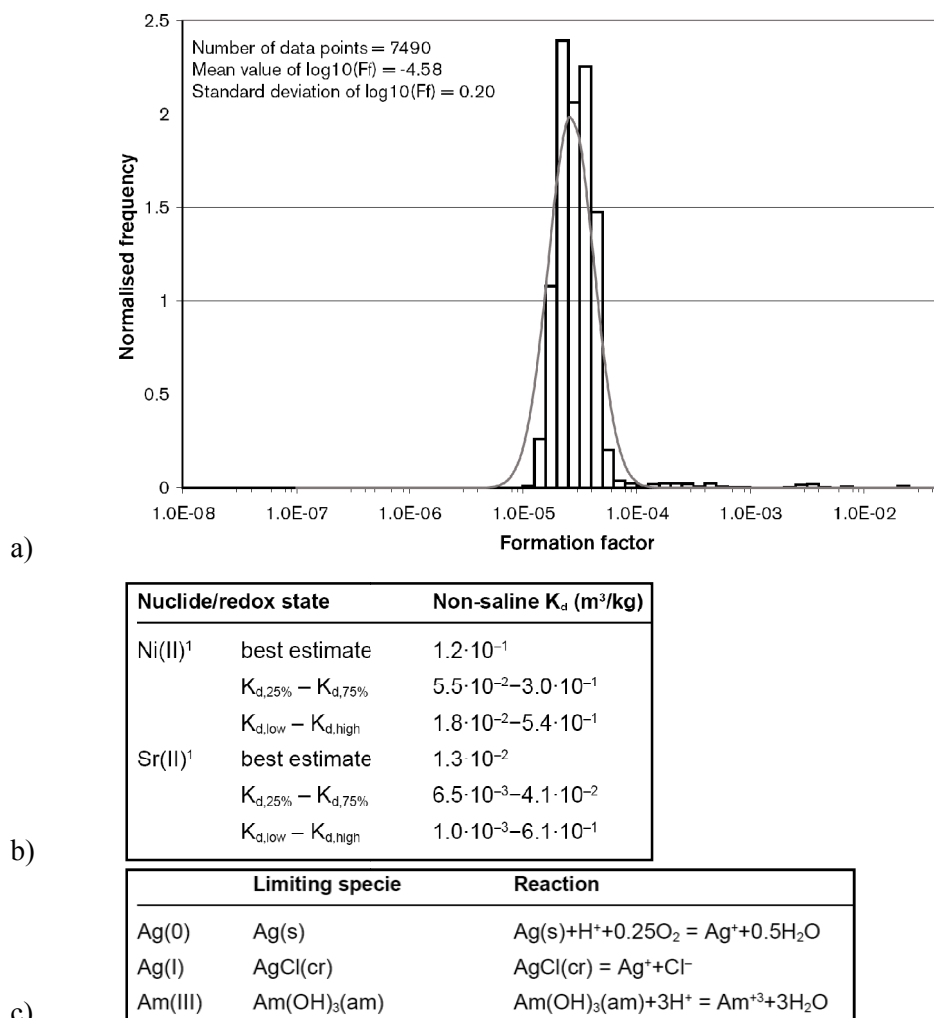


Figure 3. Examples of representations of recommended data. Reproduced from, or excerpts of, Figure 6-20, Table A-5, and Table A-43 of the SR-Can Data report.

For data which are impractical to tabulate in the Data report (for example the co-ordinates of thousands of exit locations for groundwater flowpaths), it is sufficient to precisely refer to a database or equivalent. However, if possible the data should be illustrated in figures or excerpts of tables.

2.11 Judgements by the SR-Site team

In this section, the customer representative, on behalfs of the SR-Site team, should document the examination of the delivery provided by the supplier, and make judgment on the data qualification process and on the qualified data. This text should be produced in close cooperation with persons of the SR-Site team with special knowledge and responsibility. In case of unresolved issues, the final phrasing should be decided upon by the SR-Site team.

2.11.1 Instructions to the customer representative and SR-Site team

The customer representative should make comments on all the sections listed below:

- Sources of information and documentation of data qualification.
- Conditions for which data are supplied.
- Conceptual uncertainty.
- Data uncertainty due to precision, bias, and representativity.
- Spatial and temporal variability of data.
- Correlations.
- Results of supplier's data qualification.

If appropriate, a response to the section "Supplier input on use of data in SR-Site and SR-Can" may also be warranted.

Concerning the section "Sources of information and documentation of data qualification" the customer should judge if appropriate documents are referenced, and if the categorisation of data sets into qualified or supporting is adequately performed and justified.

Concerning the section "Conditions for which data are supplied" the customer should focus upon whether the conditions given by the supplier are relevant for SR-Site modelling. If not, it should be accounted for how this is handled in SR-Site (for example by extrapolating data, using generic data, or assuming pessimistic values) and what degree of uncertainty such a procedure induces.

Concerning the section "Conceptual uncertainty" the customer should judge whether the discussion provided by the supplier is reasonable and sufficiently exhaustive. If the customer sees the need to include additional sources of conceptual uncertainty, such should be described and if possible quantified. Finally, where necessary the impact of the conceptual uncertainty on the assessment should be discussed, as well as how conceptual uncertainty is handled in SR-Site modelling (for example by applying pessimistic corrections factors to the data).

Concerning the section "Data uncertainty due to precision, bias, and representativity", the customer should make a judgment on the account provided by the supplier. Also, if the customer sees the need to include additional sources of data uncertainty, these should be described and if possible quantified. If necessary the impact of the data uncertainty on the assessment should be discussed, as well as how data uncertainty is handled in SR-Site modelling (for example by applying data uncertainty distributions or using corrections factors for the data).

Concerning the section "Spatial and temporal variability of data" the customer should focus upon whether the spatial and temporal variability are adequately characterised and whether they are of relevance for SR-Site modelling. Also, if the customer sees the need to include additional sources of spatial and temporal variability, such should be described and if possible quantified. In necessary, the impact of the spatial and temporal variability on the assessment should be discussed, as well as how this is handled in SR-Site modelling (for example by applying data distributions or different data for different model times and volumes).

Concerning the section “Correlations” the customer should scrutinise the correlations and functional relationships suggested by the supplier. Also, if correlations other than those suggested by the supplier are identified in the SR-Site project (for example in Process reports) these should be briefly described where necessary. If appropriate, a summary could be provided concerning which correlations are of actual importance for safety assessment modelling and results.

Concerning the section “Result of supplier’s data qualification” the customer should make judgement on the choice of data by the supplier, based on scientific adequacy, usefulness for the safety assessment, and the data qualification process. Comments could be made on the delivered estimates of data uncertainty and natural variability, as well as on the data reinterpretation/refinement/reduction process. Furthermore, the delivered distributions, data ranges, etc. should be scrutinised from a statistical point of view. It should be judged whether the suggested way of representing data, for example by a log-normal distribution, is adequate for SR-Site modelling. If the SR-Site team chooses to promote other data than those suggested by the supplier, the choice should be fully documented.

For all the sections listed above, supplier statements or supplied data believed to be extra uncertain, dubious, or even erroneous should be highlighted by the customer. These matters should be raised with the supplier and, if possible, resolved and accounted for in this section.

2.12 Data recommended for use in SR-Site modelling

The main delivery of the Data report to the SR-Site modelling is recommendations of data that generally are numerically well defined. Such recommended data should be given in this section.

2.12.1 Instructions to the customer representative and SR-Site team

Based on all the available information, but also on the needs from SR-Site modelling, the customer representative and SR-Site team should make a final choice of data in form of well-defined probability distributions, including natural variability, data uncertainty and other uncertainty. The choice should be fully documented and the resulting data should be tabulated. Also guidelines for how to use the data in subsequent modelling should be given, as required. Justifications and guidelines should be kept short so that this subsection mainly contains tabulated data that are easily extractable for the SR-Site safety assessment modelling.

In the process of making the final choice of data, the supplier representative, and potentially also other members of the supplier team, will be consulted one more time in a data qualification meeting. Here the formal decision on the data recommended for use in SR-Site modelling should be taken, and records of the meeting should be made as part of the SKB quality assurance system. The formal decision should be acknowledged by those representing the supplier team and those representing the SR-Site team.

The main delivery of the Data report to the SR-Site modelling is recommendations of data that generally are numerically well defined. Such recommended data should be given in this section. Based on all the available information, but also on the needs from SR-Site modelling, the customer representative and SR-Site team should make a final choice of data in form of single point values, ranges, or well-defined probability distributions, encompassing natural variability, data uncertainty, and other uncertainty. These data should be clearly tabulated (or otherwise presented) in this section. Alternatively, precise referencing to tables or equivalent in previous sections can be made. For data which are impractical to tabulate in the Data report it is sufficient to precisely refer to a database or equivalent.

Also short guidelines for how to use the data in subsequent modelling should be given, as required. Justifications and guidelines should be kept short so that this section mainly contains tabulated data that are easily extractable for SR-Site safety assessment modelling.

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Register of revisions

Version	Date	Content of revision	Made by	Reviewed by	Approved by
4.0	2011-05-05	<p>Section 1.4: It is redefined who approves the data qualification meeting protocol (and ultimately the data). It is now stated that individual authors are listed in the SR-Site expert list and not the Data report. There are small changes on the routines concerning data qualification meetings.</p> <p>Section 2: Figure 1 is exchanged to better reflect the actual stages of the preparation of the data report. Associated descriptions are modified correspondingly.</p> <p>Sections 2.1, 2.5, 2.6, 2.8, 2.9, 2.11, 2.12: Non-essential changes in wording to reflect that of section 2.3 in the Data report.</p> <p>Section 2.2, 2.3: A few of the demands on the customer are softened, to reflect section 2.3 in the Data report. Also non-essential changes in wording.</p> <p>Section 2.4: A few</p>	Martin Löfgren		

		<p>of the demands on the supplier are softened, to reflect section 2.3 in the Data report. Also non-essential changes in wording and structure.</p> <p>Section 2.7: A few of the demands on the customer are softened, to reflect section 2.3 in the Data report. Also non-essential changes in wording. Figure 2 moved to here.</p> <p>Section 2.10: Substantial modifications with the aim at softening the demands on the supplier, and to reflect section 2.3 in the Data report.</p>			
3.0	See head of the first page	<p>Section 1.4 has been entirely re-written to better describe the practical application of the instruction.</p> <p>The roles of different parties, including who finally approves the data, have been clarified.</p>	Martin Löfgren Fredrik Vahlund	See head of the first page	See head of the first page
2.0	2008-10-20	<p>Editorial changes: <i>Level 4 headings in subsection 2.1.1 (Defining the data requested from the supplier & SR-Site modelling activities in which data will be used) subsection 2.2.1</i></p>	Martin Löfgren Fredrik Vahlund	Christian Nyström	Allan Hedin

		<i>(Conditions for which data were used in SR-Can, Sensitivity to assessment results in SR-Can, Alternative modelling in SR-Can)</i> <i>subsection 2.4.1 (Sources of information, Categorising data sets as qualified or supporting data, Qualified data, Supporting data)</i> and unifying level 4 fonts.			
1.0	2008-10-14	New document	Martin Löfgren Fredrik Vahlund	Christian Nyström	Allan Hedin