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Plan for model and data quality assurance for the SR-Site project

Appendix 3 to 1064228 – SDK-003 Quality assurance plan for the safety assessment SR-Site

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1 Introduction and application of the plan

This document gives an overview of QA instructions related to the handling of model calculations and input data for the safety assessment SR-Site. The document is part of the SR-Site quality assurance plan, [1064228 - SDK-003 Quality assurance plan for the safety assessment SR-Site](#). The document provides an introduction to applicable QA routines to anyone responsible for computational tasks in SR-Site.

In the assessment project SR-Site, numerous computational tasks are performed. This involves, for instance, testing of different hypothesis, calculation of input data or performance and migration calculations. The computational tasks are identified in an Assessment Model Flowchart, AMF, which illustrates, graphically, how the tasks are related and how data are passed. In addition to the tasks identified in the AMF, other kinds of calculations are also performed within the framework of the safety assessment project. This involves, for instance, conversion of units, pre- and post-processing of data or other kinds of simpler, easily verified calculations. These simpler calculations are, although necessary for the assessment, not regarded as assessment calculations and hence not covered by the QA routine. This is further discussed in the instruction [1082130 - SR-Site MSR Instruction](#).

Important objects used for model and data QA are (each described below in Chapter 4-12):

- **The Assessment model flowchart**, in which data and models are identified. Instruction for producing the AMF is described in [1082130 - SR-Site MSR Instruction](#).
- **Process reports**, these are vital for code QA as the processes important for long-term safety are identified and evaluated. QA routines for these are presented in separate documents, [1082127 - Instruction for developing process descriptions in SR-Site and SR-Can](#).
- **Design and production reports** define the initial state of the repository and hence provide important input data for many of the computational tasks. QA routines for these are presented in separate documents.
- **The Data report** presents data used in the assessment together with discussions on and quantifications of associated uncertainties. Assessment model flowcharts are used to identify the data that are to be included in the Data report. A separate instruction, [1082129 – Supplying data for the SR-Site data report](#), exists for qualifying data for the assessment.
- **The Data storage** is used to store data that are, for any reason, not suitable to include in the Data report in the desired format. Data in the Data storage may however appear in the Data report (or other reports) in other formats. Geographical information is for instance best displayed when plotted on maps and vast number of data points may preferably be presented in histograms. The Data storage runs under a version control system which allows for revisions of the data sets to be stored.
- **The Model summary report** presents all codes (identified from the Assessment model flowchart) used in the assessment. In the Model summary report rationales for choosing a certain code are given as well as the formal decision to use the code for assessment calculations. A separate instruction, [1082130 - SR-Site MSR Instruction](#), exist for qualifying models for use in the assessment.
- **The Model storage** is a centralised storage area where models, source codes and other kind of files, like Excel spreadsheets, are stored. The model storage is version controlled so that all revisions of a specific file could be obtained. As some codes are used and owned by contractors, it is not required to store codes in the Model storage.
- **The Task description** is an instruction describing how computational tasks should be performed. In the task description, input data, methods to be used in the calculations and expected results are specified. The task description is described in the instruction [1183027 - Task description for the safety assessment SR-Site](#).
- **The Analysis documentation** is used for presenting results of computational tasks in the calculation reports. A template is provided for the analysis documentation. There exists no separate instruction for the Analysis documentation and following the analysis documentation is not mandatory.

- **Control of data used in calculations/modelling tasks, [1186612 - Final control of data used in SR-Site calculations/modelling](#)**, is an instruction used to ensure that data that are used in the final analysis agrees with those in supporting documents. The reason for this is that the complex analysis with numerous dependencies between calculations requires non-qualified data to be used in early parts of the analysis.
- **The Issue tracking system** is used mainly for code development but also in combination with the Data storage where errors in codes and data are reported. There exists no separate instruction for the Issue tracking system and using the Issue tracking system is not mandatory.

In the following sections each of the above objects is described in more detail.

2 Objective

The purpose and objective of this plan is to provide an overview of quality assurance routines related to data and models used in the safety assessment SR-Site. The plan also refers to other important instructions related to data and models.

3 Scope

This plan applies to all handling of data and models and to all calculations and modelling work in the safety assessment SR-Site. It applies both to the SR-Site project team and to suppliers to the project, from within SKB and from external suppliers.

4 Assessment model flowchart

In Assessment Model Flowcharts, AMFs, modelling activities, input and output to and from the activities and assessments based on model output are identified for different parts of the repository system (fuel/canister, buffer/deposition tunnel backfill, geosphere and external). Due to the nature of the safety assessment project, the AMFs will be continuously updated, as described in [1082130 - SR-Site MSR Instruction](#), and the final versions will appear at the final stage of the project.

For the SR-Can Assessment /SKB, 2006/, two AMFs were produced, one representing modelling tasks during the excavation, operation phase and the initial temperate period, and a second where modelling tasks performed for the permafrost and glacial conditions were presented. These two AMFs serve as baseline AMFs for the SR-Site project.

The teams behind the Model summary report and the Data report are responsible for keeping the AMFs updated.

5 The Data report

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. Instructions for qualifying data for the assessment are presented in a separate document: [1082129 – Supplying data for the SR-Site data report](#). The text below is a brief summary of that instruction.

Data should be assessed through standardised procedures, adapted to the importance of the data, aiming at identifying the origins of uncertainties and distinguish between input and judgements made by the assessment team. However, there are several issues related to data that are not covered in the Data report. Evaluation of processes and selection of models fit for use in the assessment process will be made in the 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 Main report. Design and production reports define the initial state of the repository. Descriptions of the sites will be given in the Site descriptive reports. The Data report will be based on the judgements made in those reports and does not repeat information given there, unless it is needed for the further assessment of the information or for readability. However, additional judgements will sometimes be needed, in order to define input data in a form appropriate for use in the assessment.

As the Data that should be presented in the Data report (data inventory) are based on the scenario selection in the Main report and the models presented in the AMFs, the final data inventory will not be

complete until late in the project. The updated AMF and input from the SR-Site team throughout the project will, however, provide sufficient information for producing the Data report. The Data report team is responsible for the Data report.

6 The SR-Site Data storage

The Data report can not, due to the large amount of data, be the only source of qualified data for the assessment. For instance, in the SR-Can assessment, the hydrogeological simulation resulted among many things in discharge points where radionuclides potentially could reach the biosphere. These, approximately 10,000 discharge points, were given as coordinates in the RT90 system and were easily plotted on a map. Transferring these to the biosphere assessment code was, although trivial, a potential source for errors in the analysis. Therefore, a centralised storage area where data could be exchanged is required.

All data stored in the storage have to be controlled and approved for use in a corresponding way as all data used in the analysis (see Chapter 5). All data in the storage should be well described including a reference to corresponding chapter in the Data report. The user of the data is responsible for using the latest dataset and for converting the data into a suitable form for analysis, how this is done is described in the task description, Chapter 6.

Responsible for the Data storage is the Data report team. Decision on which data to be stored in the repository is made by the Data report team and the data supplier.

7 The Model summary report

The Model summary report covers the QA requirements for computer codes and mathematical models. Instructions for qualifying codes for use in the assessment are given in a separate document, [1082130 - SR-Site MSR Instruction](#). The text below is a brief summary of that instruction.

The document produced according to the routine includes:

- Assessment model flow charts (AMFs) which are used to describe how the modelling tasks in the assessment are related and which data are passed between the models. QA requirements for the AMF are given earlier in the present document.
- A text describing the principles behind the QA measures for computer codes and calculations in the assessment. This text is summarised in a template which is used when presenting the codes. This text may be written by the user of the code.
- A presentation of each code used for modelling tasks identified in the AMF, with references to other documents that describe the mathematical model (the equations solved), verification measures, QA routines for input data handling and storage of results, QA routines for code development, version control, etc. This text may be written by the user of the code.
- A presentation of how data are passed to and from the model. This text may be written by the user of the code.
- A formal decision to use the code for assessment calculations.

The aim of the Model summary report is, however, not to discuss whether a certain process should be included in the modelling or to defend the selected input data. This is done in separate Process reports and the Data report. Moreover, as results of the computational tasks and the methodology used when performing the calculations are presented in separate documents, discussions on the accuracy in the results and other modelling related tasks are naturally also carried out in these documents.

The Model summary report team is responsible for the Model summary report.

8 The Model storage

The model storage is a source controlled storage area for storing codes. In the storage, code development and modifications should be conducted such that older versions can be reconstructed. The Model storage is based on Subversion and allows for both text based models as well as binary files to be version controlled. Hence, models from different sources like text macros, Excel spreadsheets and compiled codes may be stored at the same location. All models that are stored in the Model storage should be

stored in “ready to run” directories allowing for easy configuration on different host platforms. It is suggested that tagging and branching are used extensively to enhance the transparency in the analysis work. Decisions on which models that are stored in the Model storage are made by the customer of computational work and specified in the task description, Chapter 9.

From a source control perspective there is no difference between the Data and the Model storages, the only reason why these are treated under different sections in this document is to highlight the difference from the user perspective.

The Model summary report team is responsible for the Model storage.

9 SR-Site Task description

The task description, [1183027 - Task description for the safety assessment SR-Site](#), contains information on how the computational tasks should be conducted. The task description is jointly written by the supplier of the computational task and the customer ordering the task and should address the following issues:

9.1 Introduction and objectives

In this part of the task description, the objectives and scope of the computational task are described. This includes a discussion on the boundary conditions, conceptual models to be used as well as potential sources of error and assumptions for the task.

9.2 Approach

In this part of the task description the approach for the computational task is described as well as requirements on quality assurance. If defining the approach is part of the task this is indicated in this section.

9.3 Input data

In this section, the input data and, if stored on central locations, how to get access to the data are presented. If defining input data is part of the task this is indicated.

9.4 Software list and handling of configuration and scripting files

In this section, issues related to the software to be used in the analysis are presented and also how scripts and, if applicable, codes used in the analysis should be stored for future use.

9.5 Deliverables and output data format

In this section, deliverables from the computational task is presented. This includes format for output data and which data that should be made available.

10 The Analysis documentation

The results of the calculations are reported in a calculation report which is written by the persons performing the calculations. The report should be written so that a qualified person could reconstruct the work and reproduce the results. The exact outline is not prescribed (this is done in the Task description) but the report should include topics as:

Description of the problem

A description of the problem, including an explanation of the scientific approach, including:

- Discussion and a sketch of the grid, if the problem was spatially discretised.
- Boundary and initial conditions.
- The time period of analysis.
- Any other aspects of the approach needed to provide traceability and reproducibility.

Description of the code and input files that were used

- A description of the code including hardware, operating system and how the system was configured.
- All files (macros and input files) that are needed to reproduce the result.
- Software QA system used, for instance source control systems and issue tracking systems.

Input data

A description of the input data and how input data are transformed into code specific input.

- Each parameter and a brief description.
- Identification and discussion on variables used for numerical control and solvers used. Note that this text should also include hard-wired data.
- How other data was input into the model, for instance by using the SR-Site Data storage.
- For data not given in the Data report or from the Data storage, a discussion of the origin of the data and uncertainties therein.

Results and discussion

A description of the work performed and the results obtained including:

- Tables, plots and discussion of results. The text should provide sufficient details to demonstrate to an equally qualified technical person that the results of the analysis adequately meet the purpose of the analysis.
- Discussion of other items necessary for traceability, transparency and reproducibility.

11 Control of data used in calculations/modelling tasks

The instruction [1186612 - Final control of data used in SR-Site calculations/modelling](#), provides a procedure for final control of data used in calculations/modelling against qualified data in the data report and other supporting documents and for documentation of the control. Such a procedure is needed since the complex analysis with numerous dependencies between calculations requires that non-qualified data are used in early parts of the analysis.

12 Issue tracking system

In the issue tracking system, bugs in the code, errors in input data and other issues may be reported. The issue tracking system keeps track of the version of the code and input data that the issue are related to and provides a front-end to the Data and Model storage. In the system, full revision history of the codes, the data and assigned tasks are available at a central location. There exists no separate instruction for the Issue tracking system and using the Issue tracking system is not mandatory.

13 References

SKBdoc 1082130 - SR-Site MSR Instruction

SKBdoc 1082127 - Instruction for developing process descriptions in SR-Site and SR-Can

SKBdoc 1082129 – Supplying data for the SR-Site data report

SKBdoc 1183027 - Task description for the safety assessment SR-Site

SKBdoc 1186612 - Final control of data used in SR-Site calculations/modelling

SKB 2006, Long-term safety for KBS-3 repositories at Forsmark and Laxemar – a first evaluation Main report of the SR-Can project. SKB TR-06-09, Svensk Kärnbränslehantering AB.

14 Register of revisions

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1.0	See head of the first page	New document	Fredrik Vahlund	See head of the first page	See head of the first page

