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Instruction

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Author Fredrik Vahlund			Date 2007-08-29	
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SR-Site Model summary report instruction

Part of SDK-003, Quality assurance plan for the safety assessment SR-Site

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Svensk Kärnbränslehantering AB

Swedish Nuclear Fuel and Waste Management Co

PO Box 250, S-101 24 Stockholm

Visiting address Blekholmstorget 30

Phone +46-8-459 84 00 Fax +46-8-661 57 19

www.skb.se

556175-2014 Seat Stockholm

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1 Introduction and application of the instruction

The purpose of this instruction is to describe how code related Quality Assurance, QA, issues should be handled in the assessment project SR-Site and how this should be reported in the Model summary report. This instruction contains a description of the chosen methodology for model QA and a template to be used when writing text addressing model and code QA issues in the Model summary report.

1.1 Objective and scope of the instruction

The objective of this instruction is to provide information on how codes should be described in the Model summary report. This instruction is part of the 1064228 – Quality assurance plan for the safety assessment SR-Site and it applies to all supplier of text for the SR-Site model summary report.

1.2 Organisation of the document

The purpose of the instruction is presented in this chapter, and the basic ideas for code documentation and requirements on codes used in the assessment calculations are described in Chapter 2. To identify the codes, Assessment Model Flowcharts, AMFs, are used. While some tasks are simple scoping calculations other require complex computer codes. As it would be impractical to include all kinds of calculation tasks and to apply the same requirements on all codes, the codes are subdivided into categories, presented in Chapter 2, for which the requirements are formulated differently. The requirements on codes used for the calculation tasks are described in the Chapter 3 together with a template to be used when describing each code.

2 Principles for quality assurance of computer codes

In this chapter, principles relating to quality assurance of computer codes for the assessment project SR-Site are described. The different codes used in the assessment will, together with the chosen methodology, be presented in a Model summary report. AMFs provide an overview of all major models used in the assessment and the flow of information between them (either results or input data). Thus, the AMF identifies the different codes to be used in the assessment. For each code, QA requirements are then defined and a template for documenting how these QA requirements apply for different codes is presented.

2.1 Objective of the model summary report

The model summary report is one of the main references to the SR-Site assessment and covers QA measures for computer codes and mathematical models. The report will include:

- Assessment model flow charts (AMFs) which are used to (graphically) describe how the different modelling tasks in the assessment are related and which data are passed between the models. The AMFs are then used to identify the model and data inventory for the Model summary report and the Data report, respectively.

- A text describing the principles behind the chosen QA requirements and a template to be used when the different codes are presented in the SR-Site model summary report (see bullet point below).

- A presentation of each code used for modelling tasks that have been identified from the AMF. The text includes references to documents that describe the mathematical model (the equations solved), verification studies that have been performed, routines for input data handling and storage of results, QA routines for code development, version control, etc.

The aim of the Model summary report is, however, not to discuss the validity of the chosen models or to defend the selected input data. This is done in the Process reports and the Data report. If other models or

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data than the suggested have been used for reasons like computational conveniences or available models etc., rationales for doing this and the validity of the chosen model or data must, however, be addressed in the calculation reports and in the Model summary 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 related tasks are naturally also carried out in calculation reports.

2.2 Assessment model flow chart

For the SR-Can Assessment, /SKB, 2006/ two different AMFs for the modelling tasks were produced; one for the excavation, operation phase and the initial temperate period, and a second for permafrost and glacial conditions. In the AMFs, modelling activities, input and output to and from the activities as well as assessments based model output are identified for different parts of the repository system (fuel/canister, buffer/deposition tunnel backfill, geosphere and external).
In addition to the models presented in the AMF, minor calculations tasks will be performed within the assessment, for instance when post-processing results or when preparing input data. These tasks and calculations are not regarded as critical for the quality of the assessment and are hence not included in the Model summary report.

2.3 Types of codes used in the assessment

A large number of modelling activities were identified from the SR-Can AMFs and several different codes were used for assessment calculations. This will also be the case in the SR-Site assessment. The complexity of the codes used ranged from simple calculations using scripts languages in commercial codes like Matlab or Microsoft Excel to large (thousands of lines) codes written in C++ or Fortran. Also the origin of the codes differed substantially from commercial or open source codes with a massive user base to codes developed in-house with the assessment project as the only user. While codes with large user base could be regarded as well tested, measures have to be taken to verify the quality of the in-house codes. For in-house and open source codes, the source codes are generally available for external review as opposed to the commercial codes where the quality assurance procedures of the developer have to be accepted. A differentiated approach to quality assurance, with adaptations to the types of codes used in the assessment, is thus required. To do this, the different codes need to be categorised, not based on the importance for the assessment results or the complexity of the code but on its origin.

The following code categories have been identified:

1. Commercial system software such as operating systems, compilers and data base software. Although necessary for the assessment, these codes are not regarded as assessment codes and are hence not included in the AMF and should consequently not be included in the Model summary report.

2. Software used to solve problems that could be verified by simple back of the envelope calculations. This category also includes codes used for unit conversion and pre- and post-processing of data. This category will not be included in the AMF and are consequently not included in the Model summary report.

3. Wide-spread commercial or open source codes. These codes have a large user base and the codes are therefore regarded to be sufficiently well tested so that the need for verification tests within the SR-Site project will be limited. Codes in this category are not written exclusively for the assessment project and the user of the code could in many cases be an expert on using the code in general. The documentation for these codes is generally extensive but not written with any particular application in mind.
   Source codes for the commercial codes are generally not available for review and the development process has been carried out independent of the SR-Site project. Using these codes naturally implies that the QA procedures applied by the code developers are accepted.

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4a Modified commercial codes. Some commercially available codes allow the user to add functionality to the original code through standardised methods and have the extension working as an integrated part of the original code. Since functionality is added, the need for verification studies of these codes is larger than for codes in the previous category. Verification studies are, however, only required for the functionality of the implemented functions and not for the original code. Usage of these codes naturally implies that the QA procedures used by the code developers are accepted, but also that good developing practices are followed for the additional parts of the code.

4b Calculations performed with codes developed in-house, frequently written in languages like C++ and Fortran. These codes are in general written with the safety assessment application in mind and have naturally a considerably smaller user base than commercial codes. The need for verification is thus larger than for the commercial codes.

There may be cases where it is not evident whether a code can be regarded as belonging to category 4a or 4b. For instance, codes developed in-house may include routines from mathematical libraries (like ODE solvers etc.) which are well tested and have a large user base. However, the basic requirement (showing that the parts of the code that is not part of the original code) is the same for the two.

The quality assurance procedures for the different categories of codes are presented in the following section. In the Model summary report, each code will be listed together with the corresponding model identified in the AMF.

2.4 Basic requirements on assessment codes

Four basic requirements regarding quality assurance of codes and calculation results apply:

1. It must be demonstrated that the code is suitable for its purpose. This is required for all categories defined above.

2. It must be demonstrated that the code has been properly used. This is required for all categories defined above.

3. It must be demonstrated that the code development process has followed appropriate procedures and that the code produces accurate results. This requirement applies to codes in category 4 since these have been developed by the implementer. For codes in categories 1 to 3, the procedures of the developer have to be accepted.

4. It must be described how data are transferred between the different computational tasks. Note that this does not include a description on how data are handled internally by the model (covered in point 1 and 2 above and in documents where the calculations are presented), instead this section addresses data transfer between modelling activities. Due to the large number of modelling activities, data could be passed between activities in many different ways. How data should be transferred may, for each modelling activity, be specified in the task description (see the instruction 1183027 - Task description for the safety assessment SR-Site).

The requirements are further described below and a template to be used when writing the code presentation for the model summary report is given in Chapter 3. Of the six headings in the template, the four middle ones relate directly to the basic requirements stated above.

3 Template for code presentation

3.1 Introduction

The code is briefly introduced and the categorisation according to the definition in Section 2.3 is given. This section should contain the following:

- A brief description of the problem solved by the code in the SR-Site assessment.

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- The usage of the code in previous performance assessments (at SKB or elsewhere) and, if relevant, which previously used code it supersedes and the reason for this.

- The version of the code and the platform used in the assessment calculations.

- The category chosen for the code based on the definition in Section 2.3, and a description of how the code has been developed.

This part may be written either by the SR-Site team or by subcontractors using the code.

3.2 Suitability of the code

It needs to be shown that the code is suitable for solving the problem at hand. One indication of suitability included in this description concerns the used input parameter ranges. The parameter ranges should be within those for which the computer code gives acceptable results. This section should contain the following information:

- A description (or references to supporting documents) of mathematical models (the equations to be solved) and a description of the methods by which the solution is obtained.

This part may be written either by the SR-Site team or by subcontractors using the code.

3.3 Usage of the code

It needs to be shown that sufficient information on the usage of the code is available. This section should contain the following:

- A description of how the code is documented. Clearly, the format of the documentation may differ considerably between different codes and is hence not specified in this QA document. In some cases, for instance spreadsheet codes in Microsoft Excel, the documentation may be included in the spreadsheet/code itself and no additional documentation is required. For commercial codes, the existing documentation is in most cases sufficient.

This part may be written either by the SR-Site team or by subcontractors using the code.

3.4 Development process and verification

For codes that have been developed for the SR-Site project (category 4) it needs to be shown that the development process has been carried out in an appropriate manner. This section should contain the following:

- The measures that have been taken to ensure that the code produces the correct solution to the mathematical problem. This can e.g. be achieved by comparison to solutions obtained with other codes or to analytic solutions for special cases, if available.

- A description of how consistency of results between different versions of the code is demonstrated. This may be done using a test batch with examples that proves the functionality of the code.

This part may be written either by the SR-Site team or by subcontractors using the code.

3.5 Handling of input data, computational results and scripts

In this section it is described how data are passed between the model at hand and other models in the AMF. In this section it is also described how results and scripts used in the calculations are archived. It is also recommended to describe how the working process is controlled, for example if the version management system Subversion SVN /Küng and Onken 2009/ is used to keep track of changes.

This part may be written either by the SR-Site team or by subcontractors using the code. Rationales for using the code in the assessment

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Under this heading, the formal decision to use the code in the assessment is provided together with a brief motivation (this text is written by the SR-Site team).

4 References:

Küng S, Onken L, 2009. TourtoiseSVN. Version: 1.6.10, Build 19898 – 32 Bit, 2010/07/16 15:46:08. Tigris.org. http://subversion.tigris.org/
SKB, 2006. Model summary report for the safety assessment SR-Can. SKB TR-06-26, Svensk Kärnbränslehantering AB.
SKBdoc 1064228 – Quality assurance plan for the safety assessment SR-Site
SKBdoc 1183027 - Task description for the safety assessment SR-Site

5 Register of revisions

Version	Date	Content of revision	Made by	Reviewed by	Approved by
1.0	2007-08-29	New document	Fredrik Vahlund	Christian Nyström (QA)	See head of the first page
2.0	See head of the first page	Minor updates based on experiences from SR-Site	Fredrik Vahlund	See head of the first page	See head of the first page

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