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Strål
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Swedish Radiation Safety Authority

Technical Note

2012:35

Review of SKB's Code Documentation and QA for the SR-Site Safety Assessment

SSM perspektiv

Bakgrund

Strålsäkerhetsmyndigheten (SSM) granskar Svensk Kärnbränslehantering AB:s (SKB) ansökningar enligt lagen (1984:3) om kärnteknisk verksamhet om uppförande, innehav och drift av ett slutförvar för använt kärnbränsle och av en inkapslingsanläggning. Som en del i granskningen ger SSM konsulter uppdrag för att inhämta information i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Syftet med detta projekt är att utvärdera SKB:s dokumentation och kvalitetssäkring av koder och matematiska modellverktyg som har använts i säkerhetsanalysen SR-Site. Granskning bör ha sin utgångspunkt i SKB:s modellrapport (SKB TR-10-51), som innehåller en översikt över alla koder som används i SR-Site. En översiktlig bedömning kring ändamålsenligheten av befintlig dokumentation skall tas fram för alla koder som inkluderats i SKB:s modellrapport.

Författarnas sammanfattning

Denna inledande granskning undersökte dokumentation och kvalitetssäkring av koder som använts av Svensk Kärnbränslehantering AB(SKB). En sådan dokumentation och kvalitetssäkring är viktig för säkerhetsanalysen SR-Site eftersom datorkoder måste dels vara lämpliga för de analyser som behöver genomföras, dels kapabla att producera noggranna resultat för dessa analyser. SKB har tagit fram en rapport som sammanfattar den dokumentation av koder som finns tillgänglig för användarna och de kvalitetssäkringsrutiner som har tillämpats för dessa koder. Granskningen för att avgöra om SKB:s dokumentation av koder samt kvalitetssäkring är tillräcklig fokuserade på SKB:s sammanfattningsrapport över koder (SKB "Model summery report", SKB-10-51) samt andra dokument som identifieras i sammanfattningsrapporten.

SKB har använt 22 koder i sitt arbete med att ta fram säkerhetsanalysen SR-Site. Sammanfattningsrapporten går igenom tre kategorier: (i) kommersiella koder: ABAQUS, CODE_BRIGHT, ConnectFlow, Ecolego, ERICA Tool, MATLAB, MIKE SHE, PHAST, PHREEQC och TOUGHREACT; (ii) modifierade kommersiella koder: 3DEC, ABAQUS och CODE_BRIGHT; och (iii) projektspecifika koder: Analytisk modell för kvantifiering av buffert erosion och kapsel korrosion, Darcy Tools, FARF31, MARFA, MATLAB_COMP23, MATLAB-FPI, MATLAB-Pandora, Numerisk GIA modell, Numerisk Permafrost modell, Löslighetsmodell (Enkla Funktioner), och UMISM. SKB har använt flera versioner av samma koder och har infört flera modifieringar av de kommersiella koderna för deras användning.

En slutsats av denna granskning är att mängden tillgänglig information och värdet av tillgänglig information varierade betydligt bland de koder som granskats. Vissa koder är väldokumenterade och tillgängliga dokument bidrar till ett stort förtroende att koderna är lämpliga och kapabla att utföra erforderliga analyser. Den tillgängliga informationen kopplad

till ungefär hälften av de koder som undersökts beskriver däremot inte tydligt hur koden visats kapabel att generera noggranna resultat. Några koder uppfyller dessutom inte SKB:s egna krav för att utveckla koder som tagits fram för att säkerställa att koderna fungerar som avsett.

Granskarna rekommenderar att SKB bör ta fram erforderlig information för att bibringa en större tilltro till att koderna producerar tillförlitliga resultat.

SKB bör klargöra grunden för sin slutsats att de kommersiella koderna ERICA tool, PHAST, PHREEQEC, och TOUGHREACT som används i säkerhetsanalysen SR-Site producerar tillförlitliga resultat. Sammanfattningsrapporten för koder identifierar inga referenser eller annan specifik information som understödjer en verifiering av dessa koder. SKB bör dessutom klargöra grunden för sin slutsats att de projekt specifika koderna Analytisk modell för kvantifiering av buffert erosion och kapsel korrosion, MATLAB-FPI, MATLAB-Pandora, Numerisk GIA modell, Numerisk permafrost modell, Löslighetsmodell (Enkla funktioner) och UMISM producerar tillförlitliga resultat. SKB bör ta fram ett klart samband mellan varje användning av en specifik kod i SR-Site med information kopplad till verifiering och validering. Ett sådant klargörande är nödvändigt för att öka tilltron till att de koder som används i SR-Site har kapacitet att generera tillförlitliga resultat.

SKB bör där så är tillämpligt klargöra hur information i sammanfattningsrapporten för koder och dess referenser gäller för de olika versionerna av koderna som använts i SR-Site. Detta klargörande behövs eftersom varje enskild version av en kod behöver var för sig visas producera korrekta resultat.

Granskarna rekommenderar också att SSM bör genomföra ytterligare granskning för att stärka tilltron till resultaten från SKB:s koder.

Projektinformation
Kontaktperson på SSM: Bo Strömberg
Diarienummer ramavtal: SSM2011-4243
Diarienummer avrop: SSM2011-4546
Aktivitetsnummer: 3030007-4025

SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) reviews the Swedish Nuclear Fuel Company's (SKB) applications under the Act on Nuclear Activities (SFS 1984:3) for the construction and operation of a repository for spent nuclear fuel and for an encapsulation facility. As part of the review, SSM commissions consultants to carry out work in order to obtain information on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

The objective of this project is to make an assessment of SKB's documentation and quality assurance of codes and mathematical modeling tools used within the SR-Site safety assessment. The review should as a starting point focus on the Model summary report (SKB TR-10-51), which is an overview of all codes used in the SR-Site safety assessment. A brief assessment of the sufficiency of code documentation shall be made for all codes included in the Model summary report.

Summary by the authors

This initial review examined the Swedish Nuclear Fuel and Waste Management Company (SKB) code documentation and quality assurance, which is important to the safety assessment SR-Site because the computer codes used must be both suitable for the analyses performed and capable of producing accurate results for those analyses. SKB has prepared a report that summarizes the code documentation available for the codes used and the quality assurance processes applied to those codes. The review to determine whether SKB's code documentation and quality assurance is adequate focused on SKB's model summary report (MSR) and other documents that are identified in the MSR.

SKB used 22 codes in developing its safety case in SR-Site. The MSR addresses three categories: (i) commercial codes: ABAQUS, CODE_BRIGHT, ConnectFlow, Ecolego, ERICA Tool, MATLAB, MIKE SHE, PHAST, PHREEQC, and TOUGHREACT; (ii) modified commercial codes: 3DEC, ABAQUS, and CODE_BRIGHT; and (iii) project-specific codes: Analytical model for quantification of buffer erosion and canister corrosion, DarcyTools, FARF31, MARFA, MATLAB–COMP23,

MATLAB–FPI, MATLAB–Pandora, Numerical GIA model, Numerical permafrost model, Solubility model (Simple Functions), and UMISM. SKB used several versions of some codes and made several modifications to commercial codes for their use.

The review found that the amount of information and the value of the information varied widely among the codes. Some codes are well documented and the documents provide good confidence that the codes are suitable and capable to perform the analyses. However, the information for about one-half of the codes does not clearly describe how the code

is capable of producing accurate results. Also, several codes do not meet SKB standards for developing codes which if followed would assure that they perform properly.

The reviewers recommended that SKB clarify the information for the codes to provide greater confidence that the codes will produce accurate results.

SKB should clarify the basis for concluding that the commercial codes ERICA Tool, PHAST, PHREEQC, and TOUGHREACT used in the SR-Site produce accurate results. The MSR does not identify any references or specific information supporting verification of these codes. In addition, SKB should clarify the basis for determining that the project-specific codes Analytical model for quantification of buffer erosion and canister corrosion, MATLAB–FPI,

MATLAB–Pandora, Numerical GIA model, Numerical permafrost model, Solubility model (Simple Functions), and UMISM produce accurate results. SKB should provide clear correlation between each SR-Site application of a code and verification and validation information. This clarification is necessary to increase confidence that codes used in the SR-Site have the capability of producing accurate results.

SKB should provide information on whether adequate testing and defect resolution has been performed on modifications to commercial codes and project-specific code that were not developed under appropriate software development procedures. The information should include testing done to identify code defects that may adversely affect the code's ability to produce accurate results. This clarification is requested because several modified commercial and project specific codes have not been developed according to SKB's requirements to follow appropriate development pro-cedures and if inadequately tested, may have defects potentially affecting the code's ability to produce accurate results.

SKB should clarify how information in the MSR and its references applies to the various versions of a code used in the SR-Site, where applicable. This clarification is requested because each code version used should be individually shown to produce correct results.

The reviewers also recommended that SSM conduct additional reviews to gain more confidence in the results of these codes.

Project information
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Assessment

This report was commissioned by the Swedish Radiation Safety Authority (SSM). The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of SSM.

Contents

1. Introduction

On 16 March 2011, the Swedish Radiation Safety Authority (SSM) received a license application from the Swedish Nuclear Fuel and Waste Management Company (SKB) for construction of a spent nuclear fuel repository to be located in Forsmark, Östhammar Municipality, as well as to build an encapsulation facility for spent nuclear fuel in Oskarshamn. The safety report SR-Site, which was part of the submitted license application materials, is being reviewed by SSM in a stepwise and iterative fashion. The first step is called the Initial Review Phase. The overall goal of the Initial Review Phase is for SSM to achieve a broad coverage of the information provided in SR-Site and its supporting references and in particular to identify where complementary information or clarifications need to be delivered by SKB.

This technical note is part of a set of reviews for SSM by external experts to assist with the Initial Review Phase. The assignment involves reviews of SKB's code documentation and quality assurance (QA) for the codes used in the SR-Site. Reviews of code documentation and QA are important so that the suitability of codes for their intended function and their capability to produce accurate results can be determined.

1.1. Objective

The objective of the initial review is to assess the clarity, comprehensiveness, and traceability of the code documentation and QA information presented by SKB. The initial review process is designed to facilitate the main review process by identifying, in advance, parts of the SKB code information where (i) omissions or gaps in required information are present, (ii) additional or clarifying information from SKB is needed, (iii) additional detailed analyses are needed, or (iv) a more detailed assessment is recommended during the main review phase.

1.2. Approach

This initial review of code documentation and QA is structured in two parts: general examinations of code documentation and QA summaries, and more detailed examinations of a selected sample of codes.

The reviewers identified several principles that are relevant to determining whether codes are capable and suitable for their intended use.

- The suitability of a code to perform its intended function depends on the validity of the mathematical model used in the analysis. Validity may be demonstrated by previous successful use of the model for similar problems, successful simulation of laboratory and field scale experimental data, and similar methods.

- A computer code systematically developed following acceptable software QA practices should have fewer defects and more reliably generate correct results than a code developed under less controlled conditions. Such QA practices should include comprehensive code verification and validation to assure absence of coding errors.

- A code that has not been developed according to acceptable software QA practices should be evaluated to determine the extent of verification and validation necessary to adequately demonstrate that the code produces accurate results. Evidence of verification and validation may come from existing information or additional testing may be needed.

- A code that has an extensive user base and user feedback system to identify and resolve defects should have fewer defects and more reliably generate correct results. An extensive user base and defect resolution system may be considered in determining the extent of verification and validation necessary to adequately demonstrate that the code produces accurate results.

- A code not specifically developed for the SR-Site project, including commercial codes, freeware, and shareware, may not necessarily have the benefit of an extensive user base and defect resolution system. If such a code has not been developed according to acceptable software QA practices, the code should be evaluated to determine the extent of verification and validation necessary to adequately demonstrate that the code produces accurate results. Evidence of verification and validation may come from existing information or additional testing may be needed.

The code documentation and QA reviewers used the SKB Model Summary Report (MSR) (SKB, 2010) as their primary source of information for the general review. The general review consisted of a brief assessment of the code documentation and QA practices for the codes based on the summaries in the MSR. In consultation with SSM, the reviewers selected four codes, Code_Bright, CONNECTFLOW, 3DEC, and MatLab–FPI, for more detailed assessments of the MSR references for these selected codes. The codes selected for this detailed review are considered important to the SR-Site safety case and represent a cross section of commercial codes, modified commercial codes, and codes developed specifically for the safety assessment. The reviewers examined relevant documents related to those codes, such as code-related technical reports, user guides, and code qualification documents.

In a previous review related to SKB code documentation and QA, Hicks (2005) described how codes used in the SR 97 safety assessment and those planned for use in the SR–Can safety assessment had been documented and tested. Many of the codes reviewed in the Hicks report also were used in the SR–Site. The Hicks report concluded that the codes reviewed had varying degrees of documentation and recommended that SKB provide details of its software QA procedures covering different categories of software (e.g., internal, commercial, academic, and simple codes) and that user guides and verification reports should be developed for all SKB codes. The SR-Site review of code documentation and QA differs from Hicks (2005) in that the adequacy of the information developed by SKB is evaluated.

2. Review observations and discussion

2.1. Model summary report

In conducting the review for SKB code documentation and QA program implementation, the reviewers examined the MSR and selected MSR-referenced documents. The MSR includes an Assessment Model Flowchart (AMF), which identifies, for the different parts of the repository system: (i) modelling activities, (ii) input to and output from the modelling activities, and (iii) assessments based on model output. Information for 22 codes directly supporting the repository modelling activities performed in the SR-Site safety assessment is provided in the MSR.

The MSR includes four basic requirements from SKB instructions (SKB, 2007a,b) pertaining to code documentation and QA.

1. It must be demonstrated that the code is suitable for its purpose.

2. It must be demonstrated that the code has been properly used.

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 only (Modified commercial codes and Calculations performed with codes developed in-house or by SKB contractors).

4. It must be described how data are transferred between the different computational tasks.

In addition, the MSR describes a scheme for applying graded levels of code documentation and QA based on the origin of the code, as follows:

1. Commercial system software. This category includes operating systems, compilers, and database software. Although necessary for the assessment, these codes are not regarded as assessment codes and are not included in the AMF and likewise are not included in the MSR.

    The AMF identifies, for the different parts of the repository system, modeling activities, input and output to and from the modeling activities and assessments based on model output. One or more codes are used in each modeling activity. Commercial system software does not directly affect the repository modeling activities, so are not included in the AMF.

2. Software used to solve problems that could be verified by simple hand calculations. This category also included codes used for unit conversion and pre- and post-processing of data. This category also is not included in the AMF and consequently is not included in the MSR.

3. Widely used 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. The documentation for these codes is generally extensive, but not written with any particular application in mind. Using these codes implied that the QA procedures used by the code developers are accepted.

4. a) 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 for these codes is larger than for codes in the previous category. However, verification studies are only required for the functionality of the implemented functions and not that of the original code. Usage of these codes naturally implies that QA procedures used by the code developers are accepted, but also that good development practices are followed for the modified parts of the code.

    b) Calculations performed with codes developed in-house or by SKB contractors. These codes are, in general, written for the safety assessment. The need for verification of these is greater than for the commercial codes.

The discussions of the review in Sections 2.2 through 2.7 are organized around the sections of the MSR for each of the codes included:

*   Introduction—the code is briefly introduced and the code category is given.

*   Suitability of the Code—describes how the code is suitable for solving the problem at hand and that the used parameter ranges are within those for which the code solves the problem correctly.

*   Usage of the Code—shows that sufficient information on the usage of the code is available, how the code is documented, and a description of how input data and calculation results are handled.

*   Development Process and Verification—for codes that have been developed for the SR–Site project (Category 4), which describes that the development process has been carried out in an appropriate manner, including the measures that have been taken to ensure that the code produces the correct solution to the mathematical problem and a description of how consistency of results between different versions of the code is demonstrated.

*   Passing Data Between Models—a description of how data are passed between the model and other models identified in the AMF.

*   Rationales for Using the Code in the Assessment—the formal decision to use the code in the assessment is presented.

2.2. Introduction sections

The MSR sections introducing the codes adequately describe the function and category(s) of each code. The Introduction sections also identify the versions of the code used in the SR-Site.

For seven of the codes listed in the MSR, several code versions had been used in work supporting the SR-Site, but the MSR descriptions of code documentation and QA and references for a code did not differentiate among versions of the code. For example, the MSR section for CODE_BRIGHT refers to using four versions: Version 2.2 and 3beta (unmodified commercial) and two versions of SKB modifications to Version 3beta (modified commercial). The modifications to CODE_BRIGHT are discussed in Appendices C and D of Åkesson et al. (2010). However, no version numbers are identified in the body of the text of Åkesson et al. (2010). Thus, it is unclear where each version was used in the various analyses.

2.3. Descriptions of suitability of the code

The MSR contains key references that support the suitability of the code for the applications used in the SR-Site. Additional references were provided in the code 'Introduction' sections (e.g., references to precedents on the code use) and in sections on the 'Usage of the Code.' The references SKB provided in the MSR allow an assessment of code pedigree and suitability of the code application in the SR-Site.

The detailed reviews for code suitability for ConnectFlow, CODE_BRIGHT, and MATLAB-FPI provided the following observations.

ConnectFlow was used in the SR-Site to compute water flow fields in the geosphere to define pathways that could carry radionuclides to the biosphere. The reviewers noted that information in Section 3.5.2 on ConnectFlow—Suitability of the Code—is not substantial, focusing on descriptions of code features. However, key references are still provided in other sections of the ConnectFlow description to allow for evaluation of suitability of the code. The documentation by the developer, Serco, provides evidence that ConnectFlow has been used in multiple projects to address problems similar to the SR-Site.

CODE_BRIGHT was used for coupled thermo-hydro-mechanical (THM) problems. It was mostly used by SKB to deal with problems of moisture mobilization and water saturation of rock, backfill, and buffer material. CODE_BRIGHT is well documented and includes a Validation Document applying to Version 3 of the code, which includes a list of references to projects where CODE_BRIGHT has been used, thus providing robust evidence that the code has been extensively tested and accepted by the professional community.

MATLAB-FPI was used to estimate the number of canisters intercepted by fractures of a given size, based on distribution functions controlling the size and orientation of fracture planes. This computation is important, as it defines the number of vulnerable canisters that could be breached and release radionuclides to the geosphere. The MRS identifies two references providing the mathematical foundation of the method: Hedin (2011, 2008). In these papers, the number of canisters intercepted by fractures is estimated using numerical integration of distribution functions. Analytical expressions were derived for particular cases.

Munier (2010) discusses in detail the mathematical model and the implementation of the model in MATLAB. It also includes testing, benchmarking, and sensitivity cases to verify that the MATLAB code was appropriately implemented.

2.4. Descriptions of usage of the code

User manuals are generally available for all codes listed in the MSR, with a few exceptions that have no impact on code usage. Detailed reviews of CODE_BRIGHT, ConnectFlow, and 3DEC identified user manuals that covered problems (test cases), theory, constitutive basis, and user instructions for use.

MATLAB-FPI users probably used MATLAB manuals and no additional instructions should be needed. Specific observations are as follows:

- The MSR is not clear whether the CODE_BRIGHT user manual would provide adequate instructions for the modified portions of the code.

- Several Category 4 codes lack user manuals or equivalent instructions; however, code users work closely with code developers, so instruction should be available when needed (Numerical GIA model, Numerical Permafrost model, and UMISM). However, this approach makes it difficult to verify whether the code was properly used.

- Code-specific user manuals should not be necessary for MATLAB and EXCEL based codes. The MATLAB and EXCEL basic instructions should be sufficient.

2.5. Descriptions of developmental process and verification

Tables 1, 2, and 3 summarize the results of the general reviews. Separate tables are used for the three categories of codes in the MSR because different SR–Site MSR instruction requirements apply based on the code category. Additional observations from detailed reviews are included after each table when appropriate as well as discussion for each category. The reviewers noted that the information provided in the MSR and its references is not traceable to a specific version of a code where multiple versions were used for the SR-Site.

Table 1: Observations of commercial codes (Category 3)

Code	Quality assurance requirements followed during code development	Evidence for accuracy of results
ABAQUS	U.S. nuclear QA requirements	Information on web site
CODE_BRIGHT	none identified	References in MSR*
ConnectFlow	ISO 9001/TickIT	References in MSR
Ecolego	none identified	References in MSR
ERICA Tool	none identified	Affirmative statement, but no references in MSR
MATLAB	none identified	No references in MSR, but wide user base should identify and correct errors.
MIKE SHE	none identified	References on DHI† web site
PHAST	none identified	Affirmative statement, but no references in MSR
PHREEQC	none identified	Affirmative statement, but no references in MSR
TOUGHREACT	none identified	Affirmative statement, but no references in MSR

*Model Summary Report
†Danish Hydraulic Institute

Developmental process: SKB requirements for code development are not applicable to Category 3 codes; however, the MSR indicates that ABAQUS and ConnectFlow development and software management followed formal software QA programs (ISO 9001/TickIT and U.S. nuclear QA requirements). Codes that have followed recognized developmental processes should be afforded more confidence in their use.

Verification (i.e., checks to determine whether the code produces accurate results): The MSR asserts that "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." However, the MSR varies widely in the amount of verification information provided for commercial codes. For most codes, the MSR provided fairly extensive discussion and references to verification and verification activities. Conversely, the MSR provides no references for

verification for ERICA Tool, PHAST, PHREEQC, and TOUGHREACT. In these cases, the MSR does not provide adequate information to support the position that these four codes have been sufficiently well tested so that the need for verification tests within the SR–Site project will be limited.

Table 2: Observations of modified commercial codes (Category 4a)*

Code	Quality assurance requirements followed during code development	Evidence for accuracy of results
3DEC	Development process for modifications not identified in MSR†	References in MSR
ABAQUS	Development process for modifications not identified in MSR	User defined subroutines verified by using simple test examples, no references provided in MSR
CODE_BRIGHT‡	Development process for modifications not identified in MSR	References in MSR

*Several codes are in both Categories 3 and 4a. Category 4A requirements apply only to the code modifications.
†Model Summary Report
‡CODE_BRIGHT Version 3beta was used in an unmodified Category 3 and two modified Category 4a configurations.

A beta version of a code, specifically CODE_BRIGHT Version 3beta, generally indicates that the version has not been completely tested and is under a trial release to obtain user feedback and to identify defects. Use of beta versions for critical calculations is generally not desirable and should involve additional effort to identify and correct potential errors that would otherwise be expected to be avoided by using formally released (non-beta) versions.

Developmental Process: The MSR does not indicate that any of the three Category 4a codes meet SR–Site MSR instruction requirements that the code development and QA process followed appropriate procedures. The MSR instruction is not clear on how code development requirements would apply to the modifications of previously developed commercial codes.

Verification: The MSR provides adequate verification information and references for the three modified commercial codes. No verification and validation references are provided for the modified ABAQUS code, but test examples mentioned in the MSR should be adequate.

Table 3: Observations of project-developed codes (Category 4b)

Code	Quality Assurance requirements followed during code development	Evidence for accuracy of results
Analytical model for quantification of buffer erosion and canister corrosion	Excel-based code should not require a formal development process	References in MSR*
DarcyTools	MSR indicates no attempt has been made to show that DarcyTools conforms to any QA† standard	References in MSR provide comprehensive documentation of verification, validation, and demonstration
FARF31	Development procedures not identified in MSR	References in MSR includes validity document, regression tests of code changes
MARFA	NQA–1–2000‡ based software QA program	Validation tests in user manual, reference in MSR
MATLAB–COMP23	Development procedures not identified in MSR	References in MSR includes validity document
MATLAB–FPI	Development procedures not identified in MSR	References in MSR

Code	Quality Assurance requirements followed during code development	Evidence for accuracy of results
MATLAB–Pandora	Development procedures not identified in MSR	References in MSR
Numerical GIA model	Development procedures not identified in MSR	References in MSR
Numerical permafrost model	Development procedures not identified in MSR	References in MSR
Solubility model (Simple Functions)	Excel-based code should not require a formal development process	References in MSR
UMISM	Development procedures not identified in MSR	References in MSR

*Model Summary Report
†quality assurance
‡ASME, 2000

Developmental Process: The MSR provides information that MARFA code development and QA process followed appropriate procedures; however, the MSR does not indicate that any of the other Category 4b codes meet this requirement. Note that developmental process requirements should not be applicable to the three MATLAB-based codes and the Excel-based codes (i) Analytical model for quantification of buffer erosion and canister corrosion and (ii) Solubility model.

The reviewers noted that SKB instructions (SKB, 2007a,b) do not identify an appropriate code development procedure(s) for code developers to use. Appropriate procedures for code development include ASME NQA–1–2000, Subpart 2.7, Quality Assurance Requirements for Computer Software for Nuclear Facility Applications (ASME, 2000) and the ISO 9001-based TickIT Guide (British Standards Institute, 2007). Reviewers also noted that the SKB instructions had very little detail, especially compared to the accepted software development standards.

Verification: The reviewers identified good verification practices in DarcyTools, FARF31, MARFA, and MATLAB-COMP23, for which the MSR referenced "validity" and "verification and validation" documents. These documents provided evidence that verification needs for the codes were identified and appropriate verifications were performed.

The MSR provided verification references for the other codes in Category 4b; however, the extent that these references provide sufficient verifications for the SR-Site applications of the codes is not clear. In some cases, the references were not directly associated with verification of the code. For example, the MSR Section 3.13.4 relating to MATLAB-FPI identifies Hedin (2008, 2011), as references. These papers contain a mathematical model to estimate the number of canisters intercepted by fractures, which is the underlying mathematical model for MATLAB-FPI. However, the papers do not identify or refer to MATLAB-FPI or calculations performed using the code. These references are therefore not useful in demonstrating that MATLAB-FPI specifically produces the correct solution to the mathematical problem, which is the primary objective of the MSR section devoted to "development process and verification."

2.6. Descriptions of passing data between models

The information for the codes provided in the MSR adequately describes how data are passed between models, when applicable.

2.7. Rationales for using the code in the assessment

In these final sections of the MSR for each code, the results of the previous sections are considered and the formal decision to use the code in the assessment is presented. The reviewers expected that SKB would explain or justify an exceptions to the four basic requirements from SKB instructions (SKB, 2007a, b) pertaining to code documentation and QA. Exceptions to the requirements are noted in several cases, particularly as described in Section 2.5 of this report. For several codes the MSR does not identify the code development procedures required by SKB for modified commercials codes 3DEC, ABAQUS, and CODE_BRIGHT and project-specific codes Analytical model for quantification of buffer erosion and canister corrosion, DarcyTools, FARF31, Numerical GIA model, Numerical permafrost model, and UMISM. The rationales for using the code in the assessment do not provide justifications for these exceptions to stated requirements.

3. Findings

The initial review identified the following findings that are of significance to the determination whether the codes used in the SR-Site safety assessment are suitable for the intended functions and are capable of producing accurate results.

- For several codes, the MSR does not indicate that these meet the SR–Site requirements (SKB, 2007b) for code development. Specifically, the codes lacking information regarding development procedures include modifications to the three commercial codes 3DEC, ABAQUS, and CODE_BRIGHT and project-specific codes Analytical model for quantification of buffer erosion and canister corrosion, DarcyTools, FARF31, Numerical GIA model, Numerical permafrost model, and UMISM. In the reviewers' opinion, the impact of the fact that appropriate procedures were not followed in developing these codes can be mitigated by conducting sufficient verification testing to assure that code defects are found and resolved.

- The MSR does not identify sufficient information or references for concluding that the code produces accurate results for commercial codes ERICA Tool, PHAST, PHREEQC, and TOUGHREACT. Commercial codes ABAQUS, CODE_BRIGHT, ConnectFlow, Ecolego, MATLAB, and MIKE SHE appear to have been adequately verified and validated.

- The MSR and its references identify adequate verification and validation information for modified commercial codes 3DEC, ABAQUS, and CODE_BRIGHT.

- Project-specific codes DarcyTools, FARF31, MARFA, and MATLAB-COMP23 appear to have been adequately verified and validated; however, the information available in the MSR and its references does not clearly identify sufficient verification that the code produces accurate results for the codes Analytical model for quantification of buffer erosion and canister corrosion, MATLAB–FPI, MATLAB–Pandora, Numerical GIA model, Numerical permafrost model, Solubility model (Simple Functions), and UMISM.

4. Recommendations

- SKB should clarify the basis for concluding that that commercial codes ERICA Tool, PHAST, PHREEQC, and TOUGHREACT used in the SR-Site produce accurate results. The MSR does not identify any references or specific information supporting verification of these codes. In addition, SKB should clarify the basis for determining that project specific codes Analytical model for quantification of buffer erosion and canister corrosion, MATLAB–FPI, MATLAB–Pandora, Numerical GIA model, Numerical permafrost model, Solubility model (Simple Functions), and UMISM produce accurate results. SKB should provide clear correlation between each SR-Site application of a code and verification and validation information. Such clarification will increase confidence that codes used in the SR-Site have the capability of producing accurate results.

- SKB should provide information on whether adequate testing and defect resolution has been performed on modifications to commercial codes and project-specific code that were not developed under appropriate software development procedures. The information should include testing done to identify code defects that may adversely affect the codes ability to produce accurate results. This clarification is requested because several modified commercial and project-specific codes had not been developed according to SKB's requirements to follow appropriate development procedures and if inadequately tested, may have defects potentially affecting the code's ability to produce accurate results.

- SKB should clarify how information in the MSR and its references applies to the various versions of a code used in the SR-Site, where applicable. This clarification is requested because each code version used should be individually shown to produce correct results.

- SSM should conduct additional reviews to determine whether SKB clarifications are adequate and possible SR-Site document revisions provide the necessary clarity and transparency to demonstrate that codes used in the SR-Site can produce accurate results.

5. References

Åkesson, M., O. Kristensson, L. Börgesson, and A. Dueck, 2010, THM Modelling of Buffer, Backfill and Other System Components: Critical Processes and Scenarios, SKB TR–10–11, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company.

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Hedin, A., 2011, Stereological Method for Reducing Probability of Earthquake-Induced Damage in a Nuclear Waste Repository, *Mathematical Geosciences*, Vol. 43, No. 1, pp. 1–21.

Hedin, A., 2008, Semi-Analytic Stereological Analysis of Waste Package/Fracture Intersections in a Granitic Rock Nuclear Waste Repository, *Mathematical Geosciences*, Vol. 40, No. 6, pp. 619–637.

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Munier, R., 2010, Full Perimeter Intersection Criteria, Definitions and Implementations in SR-Site, SKB TR–10–21, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company.

SKB, 2010, Model Summary Report for the Safety Assessment SR-Site, SKB TR–10–51, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company.

SKB, 2007a, Instruction for Model and Data Quality Assurance for the SR-Site Project - Appendix 3 to 1064228 – Quality Assurance Plan for the Safety Assessment SR-Site (Preliminary), SKB 1082128, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company.

SKB, 2007b, SR-Site MSR Instruction (Preliminary), SKB 1082130, Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company.

Coverage of SKB reports

Reviewed report	Reviewed sections	Comments
Åkesson, M., Kristensson, O., Börgesson, L., Dueck, A., 2010. THM modelling of buffer, backfill and other system components. Critical processes and scenarios.	Skim for uses of CODE_BRIGHT	SKB TR–10–11, Svensk Kärnbränslehantering AB.
CODE_BRIGHT User's Guide, 2009	Skim	Geotechnical Engineering Department, Technical University of Catalunya, Spain.
CODE_BRIGHT v3 Validation document, 2009	All	Geotechnical Engineering Department, Technical University of Catalunya, Spain.
CODE_BRIGHT v3 Verification document, 2009	All	Geotechnical Engineering Department, Technical University of Catalunya, Spain.
Fälth B., Hökmark H., Munier, R., 2010. Effects of large earthquakes on a KBS–3 repository. Evaluation of modelling results and their implications for layout and design.	Skim	SKB TR–08–11, Svensk Kärnbränslehantering AB.
Hedin, A., 2008. Semi-Analytic Stereological Analysis of Waste Package/Fracture Intersections in a Granitic Rock Nuclear Waste Repository.	Skim	Mathematical Geosciences, 40, 619–637.
Hedin, A., 2011. Stereological Method for Reducing Probability of Earthquake-Induced Damage in a Nuclear Waste Repository.	Skim	Mathematical Geosciences 43, 1–21.
Hicks, T.W., 2005. Review of SKB's Code Documentation and Testing.	All	Galson 0333-2 Version 2, Draft 1. Galson Sciences Ltd, UK.
Munier, R., 2006. Using observations in deposition tunnels to avoid intersections with critical fractures in deposition holes.	Skim	SKB R–06–54, Svensk Kärnbränslehantering AB.
Munier, R., 2007. Demonstrating the efficiency of the EFPC criterion by means of Sensitivity analyses.	Skim	SKB R–06–115, Svensk Kärnbränslehantering AB.
Munier, R., 2010. Full perimeter intersection criteria. Definitions and implementations in SR-Site.	Skim	SKB TR–10–21, Svensk Kärnbränslehantering AB.
Olivella, S., Gens A., Carrera J., Alonso, E.E., 1996. Numerical formulation for a simulator (CODE_BRIGHT) for the coupled analysis of saline media.	Skim	Engineering Computations, 13, pp. 87–112.

Reviewed report	Reviewed sections	Comments
Serco, 2008a. ConnectFlow Release 9.6 Technical Summary Document.	Skim	SA/ENV/CONNECTFLOW/15, Serco Assurance, UK.
Serco, 2008b. NAMMU Release 9.6 Technical Summary Document.	Skim	SA/ENV/CONNECTFLOW/8, Serco Assurance, UK.
Serco, 2008c. NAPSAC Release 9.6 Technical Summary Document.	Skim	SA/ENV/CONNECTFLOW/12, Serco Assurance, UK.
Serco, 2008d. NAMMU Release 9.6 Verification Document.	All	SA/ENV/CONNECTFLOW/9, Serco Assurance, UK.
Serco, 2008e. NAPSAC Release 9.6 Verification Document.	All	SA/ENV/CONNECTFLOW/13, Serco Assurance, UK.
Serco, 2008f. ConnectFlow Release 9.6 Verification Document.	All	SA/ENV/CONNECTFLOW/16, Serco Assurance, UK.
Serco, 2008g. ConnectFlow Quality Plan.	All	SA/ENV/CONNECTFLOW/1, Serco Assurance, UK.
SKB, 2011. Long-term safety for the final repository for spent nuclear fuel at Forsmark. Main report of the SR-Site project.	Skim	SKB TR–11–01, Svensk Kärnbränslehantering AB.
SKB, 2010. Model summary report for the safety assessment SR-Site.	All	SKB TR–10–51, Svensk Kärnbränslehantering AB.
SKB, 2008. Instruction for developing process descriptions in SR-Site and SR-Can.	All	Appendix 2 to 1064228 – Quality assurance plan for the safety assessment SR-Site SKB 1082127, Svensk Kärnbränslehantering AB.
SKB, 2008. Instruction for development and handling of the SKB FEP database - version SR-Site.	4.1	Appendix 1 to 1064228 – Quality assurance plan for the safety assessment SR-Site SKB 1082126, Svensk Kärnbränslehantering AB.
SKB, 2009. Quality assurance plan for the safety assessment SR-Site.	All	SKB SDK–003, Svensk Kärnbränslehantering AB.
SKB, 2007. Supplying data for the SR-Site Data Report (Preliminary).	Skim	SKB 1082129, Svensk Kärnbränslehantering AB.
SKB, 2007. Instruction for model and data quality assurance for the SR-Site project.	All	Appendix 3 to 1064228 – Quality assurance plan for the safety assessment SR-Site (Preliminary) SKB 1082128, Svensk Kärnbränslehantering AB
SKB, 2007. SR-Site MSR Instruction (Preliminary).	All	SKB 1082130, Svensk Kärnbränslehantering AB.
SKB, 2008. Quality plan for the Spent Fuel Project.	All	SKB SDK–001, Svensk Kärnbränslehantering AB.

Suggested needs for complementary information from SKB

- Clarify the basis for concluding that the commercial codes ERICA Tool, PHAST, PHREEQC, and TOUGHREACT used in the SR-Site produce accurate results. The Model summary report does not identify any references or specific information supporting verification of these codes. In addition, clarify the basis for determining that the project-specific codes Analytical model for quantification of buffer erosion and canister corrosion, MATLAB–FPI, MATLAB–Pandora, Numerical GIA model, Numerical permafrost model, Solubility model (Simple Functions), and UMISM produce accurate results. Provide clear correlation between each SR-Site application of a code and verification and validation information. This clarification is requested to increase confidence that codes used in the SR-Site have the capability of producing accurate results.

- Provide information on whether adequate testing and defect resolution has been performed on modifications to commercial codes and project-specific code that were not developed under appropriate software development procedures. The information should include testing done to identify code defects that may adversely affect the codes ability to produce accurate results. This clarification is requested because several modified commercial and project-specific codes had not been developed according to SKB's requirements to follow appropriate development procedures and if inadequately tested, may have defects potentially affecting the code's ability to produce accurate results.

- Clarify how information in the MSR and its references applies to the various versions of a code used in the SR-Site, where applicable. This clarification is requested because each code version used should be individually shown to produce correct results.

Suggested review topics for SSM

1. Conduct an additional review to determine whether SKB clarifications are adequate and possible SR-Site document revisions provide the necessary clarity and transparency to demonstrate that codes used in the SR-Site can produce accurate results.

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

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

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