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Model summary report for the safety assessment SR-Can

Svensk Kärnbränslehantering AB

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Preface

This document gives an overview of computer codes used in the safety assessment SR-Can and the quality assurance procedures and documents relating to the codes. The safety assessment SR-Can is a preparatory step for a safety assessment that will support the licence application for a final repository in Sweden.

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Stockholm, October 2006

Allan Hedin
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Summary

This document is the model summary report for the safety assessment SR-Can. In the report, the quality assurance measures conducted for the assessment codes are presented together with the chosen methodology.

In the safety assessment SR-Can, a number of different computer codes are used. In order to better understand how these codes are related Assessment Model Flowcharts, AMFs, have been produced within the project. From these, it is possible to identify the different modelling tasks and consequently also the different computer codes used. A large number of different computer codes are used in the assessment of which some are commercial while others are developed especially for the current assessment project. QA requirements must on the one hand take this diversity into account and on the other hand be well defined. In the methodology section of the report the following requirements are defined:

- It must be demonstrated that the code is suitable for its purpose.
- It must be demonstrated that the code has been properly used.
- It must be demonstrated that the code development process has followed appropriate procedures and that the code produces accurate results.

Although the requirements are identical for all codes, the measures used to show that the requirements are fulfilled will be different for different codes (for instance due to the fact that for some software the source-code is not available for review).

Subsequent to the methodology section, each assessment code is presented and it is shown how the requirements are met.

Contents

1 Introduction

In the current chapter, the SR-Can safety assessment to which the present document is associated is initially introduced followed by a brief presentation of other documents within the SR-Can series of reports.

1.1 Objectives and scope of the SR-Can assessment

The SR-Can project is a preparatory stage for the SR-Site assessment, the assessment which will be used for SKB's application to build a final repository. The purposes of the safety assessment SR-Can are the following:

1. To assess the safety of potential KBS-3 repositories at Forsmark and Laxemar to dispose of canisters as specified in the application to build the encapsulation plant.
2. To provide feedback to design development, to SKB's R&D programme, to further site investigations and to future safety assessment projects.
3. To foster a dialogue with the authorities that oversee SKB's activities, i.e. the Swedish Nuclear Power Inspectorate, SKI, and the Swedish Radiation Protection Authority, SSI, regarding interpretation of applicable regulations as a preparation for the SR-Site project.

The assessment relates to the KBS-3 disposal concept in which copper canisters with a cast iron insert containing spent nuclear fuel are surrounded by bentonite clay and deposited at approximately 500 m depth in saturated, granitic rock. Preliminary data from the Forsmark and Laxemar sites, presently being investigated by SKB as candidates for a KBS-3 repository are used in the assessment.

1.2 Objectives and scope of the current report

The purpose of this report is to give an overview of the codes used in the safety assessment SR-Can and the quality assurance procedures and documents relating to the codes. More specifically, the report contains

- Assessment model flow charts (AMFs) that describe the modelling tasks in SR-Can and how they relate to each other.
- The principles behind the QA measures regarding the codes and the calculations.
- A brief 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

The aim is however not to present reasons for including a certain process in the modelling or to defend the selected input data. This is done in the SR-Can Process reports /SKB 2006aef/ and the SR-Can Data report /SKB 2006c/, respectively.

1.3 Organisation of the report

In the current chapter, the purpose of the report and of the SR-Can project in general is introduced. In Chapter 2, the basic ideas for the Model summary document and requirements on the codes used in the assessment calculations are presented. To do this, assessment model flowcharts, AMFs, are initially introduced in which the different calculations tasks performed in the assessment can be identified. While some of the quantification tasks identified in the AMFs are simple scoping calculations other require complex computer codes. As it would be impractical to include all kinds of calculation tasks performed and to apply the same QA requirements on all codes, the codes are subdivided into categories on which the requirements are formulated differently. The methods used for distinguishing between the different categories of codes are presented in Chapter 2. The QA requirements on codes used for the calculation tasks are also described in Chapter 2 together with a template to be used when describing each code. Finally, in Chapter 3, the different codes used for the assessment calculations are presented following the suggested outline.

1.4 Related reports

As previously indicated, the present report is one in a series of reports of the safety assessment SR-Can. The top document, in which methodology for the assessment, main results and conclusions are presented is the **Main report**[1]. In addition to the **Main report**, the SR-Can series of reports also consists a number of main references describing e.g. the initial state of the repository, three process reports describing processes in different parts of the repository system, a FEP report presenting the features, events and processes considered in the analysis. The series also consists of reports describing climate and biosphere related issues used in the analysis. The notation in Table 1-1 is used when referring to these main references.

Table 1-1. Full title and abbreviations used for documents in the SR-Can report series.

Full title	Abbreviation used in the present report	Reference
Long-term safety for KBS-3 repositories at Forsmark and Laxemar – a first evaluation Main report of the SR-Can project	**Main report**	/SKB 2006i/
Data report for the safety assessment SR-Can	**Data report**	/SKB 2006c/
FEP report for the safety assessment SR-Can	**FEP report**	/SKB 2006d/
Initial state report for the safety assessment SR-Can	**Initial state report**	/SKB 2006h/
Fuel and canister process report for the safety assessment SR-Can	**Fuel and canister process report**	/SKB 2006e/
Buffer and backfill process report for the safety assessment SR-Can	**Buffer and backfill process report**	/SKB 2006a/
Geosphere process report for the safety assessment SR-Can	**Geosphere process report**	/SKB 2006f/
Climate and climate related issues for the safety assessment SR-Can	**Climate report**	/SKB 2006b/
Handling of future human actions in the safety assessment SR-Can	**FHA report**	/SKB 2006g/

[1] Long-term safety for KBS-3 repositories at Forsmark and Laxemar – a first evaluation Main report of the SR-Can project.

2 Principles for quality assurance of computer codes

In this chapter, the principles relating to quality assurance of software and codes in the safety assessment SR-Can is described. To do this, assessment model flow charts, AMFs which provide an overview of all major models and the flow of information between them are initially presented. From the AMFs, the different computer codes used in the assessment are identified. For the different types of codes, QA requirements are identified and a template for documenting how these apply for the different codes is presented.

2.1 Assesment model flow chart

To illustrate how major modelling tasks in the assessment are related, two assessment model flow charts, AMFs, have been constructed for SR-Can, see Appendix A. The first covers modelling of the excavation and operation phase and the initial temperate period, Figure A-1, while the second covers modelling of permafrost and glacial conditions, Figure A-2. In the 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).

In addition to the models presented in the flow chart, minor calculations are performed, for instance when post processing results or when preparing input data. These tasks and calculations are not included in the present document.

2.2 Types of codes used in the assessment

The large number of modelling activities identified in the AMF indicates that several different codes are used in the assessment. The complexity of these ranges from simple calculation routines written in scripts languages in commercial codes like Matlab or Microsoft Excel to large (thousands of lines) codes written in programming languages like C++ and Fortran. Also the origins of the codes differ substantially. While some codes are commercial, have a world-wide user base and can hence be regarded as well tested, others are written exclusively for the SR-Can assessment. For codes developed within the SR-Can project, the source codes are available for external review. For the commercial codes this is not the case and 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.

The following code categories have been identified:

1. Commercial system software such as operating systems, compilers and data bases. Although necessary for the assessment, these codes are not regarded as assessment codes and are hence not included in the assessment model flowchart or in the model documentation.
2. Software used to solve problems that can be verified by simple hand calculations. This category also includes codes used for unit conversion and pre and post processing of data. This category is not included in this document.

3. Wide-spread commercial or open source codes. These codes have a large user base and the codes are therefore regarded as sufficiently well tested that the need for verification tests within SR-Can is limited. Codes in this category are not written exclusively for the SR-Can project and the user of the code may 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-Can project. Using these codes naturally implies that the QA procedures used by the code developers are accepted.

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 is larger for these codes than for codes in the previous category. Verification studies within SR-Can are however only required for the functionality of the implemented functions and not that of the original code. Using 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 part of the code developed within SR-Can.

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 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 QA compliance for the parts that is not part of the original code) is the same for the two.

Based on these categories, the quality assurance procedures for each type of code are presented in the following section. In Appendix B, each code is listed together with the corresponding model identified in the AMF.

2.3 Basic requirements on assessment codes

Three basic requirements have been formulated regarding quality assurance of codes and calculation results:

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.

The requirements and procedures used to fulfil these are further detailed below, in the form of a template to be followed when the codes identified through AMF are presented in Chapter 3. Of the five headings in the template, the three middle ones relate directly to the three basic requirements above.

2.4 Template for code presentation

2.4.1 Introduction

The code is briefly introduced and the categorisation according to the definition in Section 2.2 is given. This section should contain the following:

- A brief description of the problem solved by the code in the SR-Can application.
- The version of the code and the platform used in the assessment calculations.
- Rationales for choosing the category, the user base of the code and a description of how the code has been developed.
- 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.

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

2.4.2 Suitability of the code

It needs to be shown that 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. This section should contain the following, often through references to supporting documents:

- A description of mathematical models (the equations to be solved) and a description of the methods by which the solution is obtained.
- A description of what measures that have been taken to show that the expected parameter ranges are within those for which the computer code gives acceptable results.

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

2.4.3 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 documents 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.
- A description of how input data and calculation results are handled.

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

2.4.4 Development process and verification

For codes that have been developed for the SR-Can 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-Can team or by subcontractors using the code.

2.4.5 Rationales for using the code in SR-Can

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

3 Description of the codes

This chapter provides a listing of the codes used in the SR-Can safety assessment based on the models identified in the assessment model flowcharts. Each code and it's associated model are presented in Appendix B. The text for each code follows the outline presented in Section 2.3.

3.1 3DEC

3.1.1 Introduction

3DEC is a three-dimensional numerical program based on the distinct element method for discontinuum modelling /Itasca Consulting Group Inc 2003/.The program is based on the extensively tested formulation used by the two-dimensional version *UDEC* /Itasca Consulting Group Inc 1996/. *3DEC* simulates the mechanical and thermo-mechanical response of discontinuous media subjected to either static or dynamic loading

In SR Can, 3DEC was used for static analyses of mechanical effects on rock and rock fractures within and around the repository. Effects caused by excavation of the repository openings, by swelling pressures and pore pressures, heat generation and glacial loads were considered. Effects of particular interest were creation of stress concentrations around the repository openings and fracture displacements that may change the hydraulic conditions. Both near-field and large-scale models were analyzed. 3DEC was also used for dynamic analyses of fracture shear displacements induced by post-glacial fault movements.

For the SR-Can calculations, version 3.0 of *3DEC* was used. It was run on a Windows-based 3.6 GHz PC-system.

3DEC was originally developed for stability analyses of rock slopes. It has been used for studies related to mining engineering and for studies related to deep disposal of nuclear wastes. Both static and dynamic analyses for deep underground openings have been performed, see for instance /Stephansson et al. 1991, Sjöberg 1992, Senseny 1993/. *3DEC* has been used by SKB in studies regarding thermo-mechanical effects on the bedrock around a deep repository /Hakami et al. 1998/. Embedded in *3DEC* there is a programming language called *FISH. FISH* enables the user to define own variables and functions. *FISH* functions may be used to add new functionalities and to extend the usefulness of the code. Since *3DEC* is a wide-spread commercial code which allows the user to add functionality by use of the *FISH* language, and since specifically developed *FISH* routines are integral parts of the SR-Can application calculations, *3DEC* is regarded as a category 4a code.

Much of the rock mechanics analyses referred to in SR 97 were conducted using 3DEC.

3.1.2 Suitability of the code

3DEC is specially designed for mechanical analysis of jointed rock masses. The discontinuous medium is represented by an assemblage of discrete blocks and the discontinuities are treated as boundary conditions between the blocks. Large displacements along discontinuities and large rotations of blocks are allowed. The blocks may be either rigid or deformable. Deformable blocks are subdivided into a mesh of finite difference elements, which respond according to either linear or non-linear stress-strain laws /Itasca Consulting Group Inc 2003/. The relative displacements along the discontinuities are also governed by linear or non-linear force-displacement laws, both in the normal- and shear directions. *3DEC* also has a thermal logic implemented, which is specially oriented for solving design problems related to nuclear waste disposal. The temperatures at all node locations are calculated for specified "snapshots" in time by use of analytical point- and line source solutions. The temperatures (and temperature increments) are then used by the mechanical logic in *3DEC* for the calculation of thermal stresses. The thermal logic is based on linear thermal conduction and superposition of temperature contributions from different heat sources. The material is assumed to be thermally homogenous and isotropic with constant properties.

In the assessment work, the rock continuum, i.e. the intact rock between the discontinuities, was modelled as a linear elastic material. For the mechanical response of the discontinuities (fractures), an elastic and ideal-plastic law was applied assuming linear behaviour in the elastic range combined with the Mohr-Coulomb failure criterion.

The embedded programming language *FISH* was used for the development of a technique for defining circular-shaped fractures by assigning specific fracture material properties to selected parts of the discontinuities. This functionality was then used in analyses of seismically induced fracture shear movements. *FISH* was also used to reduce computer run time when analyzing thermo-mechanical near-field models. 3DEC temperatures were calculated once for each set of models and then imported into different model versions using the specifically developed *FISH* routines.

Parameter values used in the SR-Can applications, i.e. values of rock mass and intact rock elastic parameters, values of fracture strength and fracture stiffness as well as values of rock thermal properties, are well within ranges covered by verified examples of analyses found in the extensive *3DEC* literature.

3.1.3 Usage of the code

The documentation of *3DEC* /Itasca Consulting Group Inc 2003/ is provided by Itasca Consulting Group Inc. The documentation contains a complete description of the code and of the models that are implemented. A specific part of the documentation contains a description of the *FISH* language.

Text files containing all model data (geometries, material data, initial- and boundary conditions, solution strategies) are used as input to the code. In the input files, specific results to be monitored and recorded during the analysis can be specified. These results can be plotted or exported as text files. *3DEC* has a plotting tool, which can be used for control of the model (geometry, application of boundary conditions) during model building. The plotting tool also have a wide range of possibilities for producing vector- and contour plots used during post processing of calculation results.

3.1.4 Development process and verification

The formulation and development of the distinct element method, which is the core in *3DEC,* begun in 1971 with the initial presentation /Cundall 1971/ and the development has been in progress since then. The *3DEC* documentation includes a suite of systematic comparisons between *3DEC* results and corresponding analytical solutions. Models with different types of geometry, different types of material behaviour and different types of boundary conditions are included. At present time, the code is subject for progressive development.

The specific *FISH* routines developed for use in the safety assessment calculations were rigorously tested and verified in small test models before implementation into the assessment models.

3.1.5 Rationales for using the code in SR-Can

The SR-Can team has selected *3DEC* to be used in the safety assessment work since it is well suited for the specific problems addressed above and is also a well documented and widely used code.

3.2 Abaqus

3.2.1 Introduction

Abaqus is a wide spread commercial finite element code /Abaqus Inc/ that has been available on the market for several decades. The code is suitable for solving problems in the field of mechanical engineering, thermal transport etc. Abaqus is in SR-Can used for solving problems related to resaturation of the buffer, response to shear movement of the rock and for thermal analysis. The code is in SR-Can regarded as a category 3 code.

3.2.2 Suitability of the code

Abaqus is used for a number of tasks in SR-Can, the equation solved are further described in each modelling report.

3.2.3 Usage of the code

The documentation available for Abaqus is extensive and training classes are available at different levels.

3.2.4 Development process and validation

No dedicated verification or validation tests of the Abaqus code have been performed within the SR-Can project. A description of the QA procedures of Abaqus Inc is available on their webpage.

3.2.5 Rationales for using the code in SR-Can

The SR-Can team and the contractors involved in the modelling task consider Abaqus to be a suitable code for the applications, the code is regarded to be one of the dominating code in its field is wide spread and commonly used by the subcontractors.

3.3 Analytic radionuclide transport model

3.3.1 Introduction

The purpose of this code is to mimic the near- and far-field codes COMP23 and FARF31 through simple analytic expressions as explained in /Hedin 2002/. The simple expressions allow fast execution of probabilistic calculations, thus allowing a comprehensive calculation program in a safety assessment. The model is implemented in Microsoft Excel by the user. No rigorous version control system has been applied during the development of the code.

The probabilistic calculations are carried out with the commercially available Excel plug-in code @Risk /Palisade corporation/. This is a wide-spread tool, for which quality assurance is provided by the developer.

An earlier version of the code was used in the SR-Can Interim report /SKB 2004/. No important changes have been made to that version.

Since the code has been developed by SKB, it is of category 4b.

3.3.2 Suitability of the code

The same processes as in COMP23 and FARF 31 are modelled and justification for the conceptualisation of these is found in the references given in the description of the latter codes.

The mathematical model used in the analytic code is described in /Hedin 2002/, with a few additional details in a Note available in the SR-Can project archive. It consists of analytic expressions that are directly evaluated in Microsoft Excel.

The analytic code has been benchmarked to COMP23 and FARF31 in several exercises: i) in /Hedin 2002/, ii) in the SR-Can interim report /SKB 2004/ and iii) in the SR-Can main report /SKB 2006i/. For the latter, benchmark cases with good agreement is shown for a deterministic base case, for probabilistic base cases for each site and for a case of canister failure due to rock shear. Since the purpose is to mimic COMP23 and FARF31 and since the benchmark exercises show good agreement for the parameter ranges used in SR-Can, it is concluded that the code fulfils its purposes.

3.3.3 Usage of the code

No manual has been produced for the analytic model, and the code has been used only by the implementer. The Excel spreadsheets are not self-explanatory for an external user. A brief manual is to be developed for future assessments and the code is to be written such that it can be transferred to other users.

Input data distributions are entered in the Excel spreadsheets as an integrated part of the code. Input and output data are documented as reports generated by the @Risk plug-in used for the probabilistic executions.

A comprehensive manual is available for the probabilistic @Risk plug-in used for the probabilistic executions.

3.3.4 Development process and verification

The code consists of analytic expressions directly evaluated in Microsoft Excel, for which verification of the correctness of the mathematical solution is provided by the developer of Excel.

Consistency of results between different versions of the code is demonstrated through the repeated benchmark exercises described in the previous section.

3.3.5 Rationales for using the code in SR-Can

The SR-Can team has selected the analytic radionuclide transport model to be used in the safety assessment since it is well suited for massive probabilistic calculations while producing results similar to those obtained with the more detailed codes COMP23 and FARF31.

3.4 Analytic transport model for advective conditions

3.4.1 Introduction

The purpose of this code is to quantify radionuclide release rates from the near-field for the simple case where radionuclides are released to the rock at the same rate as they are liberated from the fuel matrix. Transport through the geosphere is modelled with a simple transmission expression. The model consists of simple analytic expressions as documented in the SR-Can main report, Appendix B /SKB 2006i/. The simple expressions allow fast execution of probabilistic calculations, thus allowing a comprehensive calculation program in a safety assessment. The model is implemented in Microsoft Excel by the user. The first version of the code is used in SR-Can.

The probabilistic calculations are carried out with the commercially available Excel plug-in code @Risk /Palisade corporation/. This is a wide-spread tool, for which quality assurance is provided by the developer.

Since the analytic code has been developed by SKB, it is of category 4b.

3.4.2 Suitability of the code

The near-field processes to model for advective conditions in the deposition hole are a small subset of those represented in the near-field model COMP23. These can be readily represented by analytic expressions as described in the SR-Can main report /SKB 2006i/. Justification for the conceptualisation of these is found in the references given in the description of the COMP23 code.

The geosphere transport processes are the same as for the FARF 31 code. As explained in /Hedin 2002/ it is pessimistic to represent these by the transmission expression given in /Hedin 2002/. The agreement with the result of the more exact solution is in general good and in particular for conditions of low transport resistance in the rock. The latter conditions are strongly correlated to advective conditions in the deposition hole as further discussed in the SR-Can main report /SKB 2006i/, thus justifying the use of this approach.

The mathematical model used in the analytic code is described in the SR-Can main report, Appendix B /SKB 2006i/. It consists of simple analytic expressions that are directly evaluated in Microsoft Excel.

The analytic code is benchmarked to COMP23 and FARF31 as documented in the SR-Can main report, Appendix B /SKB 2006i/. The benchmark case shows good agreement for a probabilistic base case. Since the purpose is to mimic COMP23 and FARF31 and since the benchmark exercise shows good agreement for the parameter ranges used in SR-Can, it is concluded that the code fulfils its purposes.

3.4.3 Usage of the code

No manual has been produced for the analytic model, and the code has been used only by the implementer. The Excel spreadsheets are not self-explanatory for an external user. A brief manual is to be developed for future assessments and the code is to be written such that it can be transferred to other users.

Input data distributions are entered in the Excel spreadsheets as an integrated part of the code. Input and output data are documented as reports generated by the @Risk plug-in used for the probabilistic executions.

A comprehensive manual is available for the probabilistic @Risk plug-in used for the probabilistic executions.

3.4.4 Development process and verification

The code consists of analytic expressions directly evaluated in Microsoft Excel, for which verification of the correctness of the mathematical solution is provided by the developer of Excel.

Consistency of results between different versions is not yet an issue since the first version of the code is used in SR-Can.

3.4.5 Rationales for using the code in SR-Can

The SR-Can team has selected the analytic transport model for advective conditions to be used in the safety assessment since it is well suited for massive probabilistic calculations while producing results similar to those obtained with the more detailed codes COMP23 and FARF31.

3.5 Ansys

3.5.1 Introduction

Ansys is a commercial finite element code /ANSYS Inc/. The code has been available on the market for several decades and can be used for solving problems in the field of mechanical engineering, thermal transport, fluid dynamics etc. The code is in SR-Can regarded as a category 3 code.

In SR-Can, Ansys has been used in different modelling tasks within the project, mainly in the area of solid mechanics but also in for thermal analysis.

3.5.2 Suitability of the code

Ansys is used for a number of tasks in SR-Can, the equation solved are further described in each modelling report.

3.5.3 Usage of the code

The Ansys code is vastly documented and training classes are offered.

3.5.4 Rationales for using the code in SR-Can

The SR-Can team and the contractors involved in the modelling task consider Abaqus to be a suitable code for the applications, the code is regarded to be one of the dominating code in its field is wide spread and commonly used by the subcontractors.

3.5.5 Development process and validation

No dedicated verification or validation tests of the Ansys code have been performed within the SR-Can project. Ansys Inc. claims however that a large number of verification tests are performed prior to each code release as part of the quality assurance routines at Ansys inc. The validity of the material models used for the buffer material and the canister shell and insert in the shear deformation simulations are discussed in the modelling report and in the SR-Can process report for the Buffer and backfill /SKB 2006a/, material properties of the canister an the buffer material is provided in the SR-Can data report /SKB 2006c/ and the modelling report.

3.5.6 Rationales for using the code in SR-Can

The SR-Can team and the contractors involved in the modelling task consider Ansys to be a suitable code for the applications, the code is regarded to be one of the dominating code in its field is wide spread and commonly used by the subcontractors.

3.6 ArcGIS and ArcView

3.6.1 Introduction

Geographic Information System, GIS, is used to manage and present geographical information and to perform logical and spatial operations on existing data to produce new data sets. One typical example of GIS use in SR-Can is to model a future costal landscape using existing maps and prediction of the shoreline displacement as a function of time. GIS data is also used as input data for other analysis, e.g. hydrology modelling. managing geographical information in data bases and to determine key parameters like sizes of different objects based on geographical representation of the sites

In the safety assessment SR-Can, GIS modelling and analysing have been performed using the codes ArcView 3.x, ArcGIS 8.x and ArcGIS 9.x, which all are products of the Environmental Systems Research Institute, ESRI Inc.

ESRI Inc. was founded in 1969 as a consulting firm specialized in land use analysis projects. 1982 ESRI Inc. launched its first commercial GIS software called ARC/INFO. Today ESRI Inc. is the world leading GIS company with 35% share of the global market, their products are widely spread and are used by more than 1 million people.

In previous safety assessments, /SKB 1995, 1999/ only generic data was used and the need for managing geographical information was limited. Therefore SR-Can is the first safety assessment performed by SKB where GIS programs have been used to a large extent.

The program is regarded as category 3 according to the previous definition.

3.6.2 Suitability of the code

Using GIS is a necessity when working with a vast amount of geographical data as in the site characterisation program. ESRI Inc. fully encompasses Open Geospatial Consortium Inc. (OGC) specifications and standards as well as comprehensive IT standards such as those related to ISO, W3C, ANSI, CEN and many other leading de-facto industry standards.

The programs have many extensions, of them Spatial Analyst and 3D Analyst adds a comprehensive set of advanced spatial modelling and analysis tools to the ArcGIS; such as spatial analysis in two or three dimensions, perform integrated raster/vector analysis and accomplish statistical analysis based on the local environment, small neighbourhoods, or predetermined zones /ESRI 2004ab/.

3.6.3 Usage of the code

ArcGIS and ArcView are commercial codes with a large user base. The codes are well documented both the codes in their original form /ESRI 2005a/ and for the extensions used in the site characterisation program /ESRI 2004ab/. In addition to the written documentation, ESRI provides training courses, traditional support, user discussion groups and a vast amount of extra documentation available on their website /ESRI 2005b/.

The data in SKB's GIS data base are purchased (e.g. from National Land Survey of Sweden (Lantmäteriet), The Geological Survey of Sweden (SGU)), gathered from authorities (e.g. from County Administration (Länsstyrelse), National Board of Forestry (Skogsvårdsstyrelsen)) and generated by the SKB site investigations. The modelling and analysis results are stored in the SKB GIS data base and published as maps and tables for reports.

3.6.4 Rationales for using the code in SR-Can

ArcGIS and ArcView are the standard GIS software for the Site Descriptive modelling project performed at SKB. Although there are other commercial codes available the SR-Can project have not consider them for use.

3.7 CodeBright

3.7.1 Introduction

CodeBright v2.2 /Cimne 2002/ is a 3D finite element program designed to handle thermo-hydro-mechanical (THM) coupled problems in geological media. The theoretical approach consists of a set of governing equations, a set of constitutive laws and a special computational approach. The code is written in FORTRAN and is composed of several subroutines. The program does not use external libraries. The code was originally developed on the basis of a new general theory of saline media, hence the name: *CO*upled *DE*formation, *BR*ine, *G*as and *H*eat *T*ransport problems. The code has been commercial for approx. five years and is regarded as a category 3 code.

3.7.2 Suitability of the code

The code solves in the most general case an initial boundary value problem consisting in a set of five governing equations (stress equilibrium, water mass balance, air mass balance, energy balance and balance of conservative solute). A Newton-Raphson iterative scheme is used to solve the non-linear system of equations.

The inclusion of a gas phase enables the explicit representation of water in both liquid and vapour form. In the same way is a gas represented both in a gas phase and as dissolved in the liquid phase.

Among the available mechanical constitutive laws, the thermo-elastoplasic law is based on the Basic Barcelona Model /Alonso et al. 1990/ which was developed to describe the hydro-mechanical behaviour of partially saturated soils. The relevance of this model for highly expansive clays is currently investigated and a subject for developments.

3.7.3 Usage of the code

The documentation of CodeBright is provided by /Cimne 2002/. The documentation contains a description of the code and the models that are implemented.

CodeBright uses GiD system for pre- and post-processing. GiD is an interactive graphical user interface that is used for the definition, preparation and visualization of all the data related to the numerical simulations. This data includes the definition of the geometry, materials, conditions, solution information and other parameters. The program can also generate the finite element mesh and write the information for a numerical simulation in its adequate format for CodeBright. It is possible to run the numerical simulation directly from the GiD system and to visualize the results without transfer of files.

3.7.4 Development process and validation

CodeBright was developed at the Technical University of Catalonia (UPC) in the beginning of the 1990s /Olivella et al. 1996/. The code has been verified and validated through comparisons with analytical solutions for a number of problems, for example (i) heat or water flow in an infinite medium from a source at constant rate; (ii) steady-state heat flow from buried pipelines; (iii) thermal-convection in a saturated medium /Olivella et al. 1996/. An analytical solution for steady-state moisture redistribution at non-isothermal conditions, with concurrent vapour diffusion and advective water flow /Claesson and Sällfors 2005/, has recently been reproduced with the code /Åkesson 2006/.

The code has also been used for predictions and evaluations of field tests at Äspö HRL, e.g. TBT /Hökmark 2005/ and Prototype /Ledesma and Chen 2005/, as well as lab-scale test /Birgersson et al. 2006/.

3.7.5 Rationales for using the code in SR-Can

CodeBright is regarded as a suitable code for solving the problem at hand. The contractor performing the calculations has a long experience in using the code.

3.8 COMP23/Compulink

3.8.1 Introduction

COMP23 /Cliffe and Kelly 2004/ is a Fortran77 code used for radionuclide migration calculations in the near-field (the canister and the engineered systems) and includes models for fuel dissolution, handling of element specific solubility, and migration through advection and dispersion in the different parts of the engineered system. The code was initially developed as NUCTRAN /Romero 1995/ and was subsequently incorporated into the SKB safety assessment calculation framework Proper as the submodel COMP23. Proper is a collection of codes used for migration and consequence calculations through the near-field, the far far-field and the biosphere and uses standardised methods to transfer data and results between the different submodels. COMP23 has been used by SKB in the SR 95 /SKB 1995/, the SR 97 /Lindgren and Lindström 1999, SKB 1999/ and the SR-Can Interim assessments /SKB 2004/ of a final repository of the KBS-3 type. A closely related code, NUCTRAN/NUCFLOW, (which origins from the same source but allows for multiple sources apposed to COMP23 which only handles single sources) was used as in the SAFE assessment of the SFR repository for operational waste /Lindgren et al. 2001/. In addition, the code has been used by Andra and, to some extent, by LEI. COMP23 has been continuously developed by SKB and subcontractors up till the present version 1.2.2. An alternative implementation of the COMP23 models is the Compulink code /Vahlund and Hermansson 2006b/ which is based on the same conceptualisation as the Fortran implementation but is written in Matlab and Simulink /The Mathworks Inc/. In SR-Can Compulink is the code used for the near-field migration calculations.

The code is considered a category 4b code.

3.8.2 Suitability of the code

COMP23 and Compulink has been developed by SKB with the main objective to solve the problem at hand and includes all essential models needed when modelling radionuclide migration through the engineered system. Some of the models have been used temporarily in the development process of the KBS-3 repository and can be regarded as being obsolete b based on the present level of knowledge. The code contains for instance several models of different complexity used to calculate the dissolution rate for the fuel matrix. However for the SR-Can a linear model will be used which corresponds best to the present level of knowledge of the actual processes /Werme et al. 2004/ suggested in the Data report and the Fuel and canister process report. For the solubility limits inside the canister which is a mechanism limiting the concentration inside the canister, a shared solubility model will be used where the solubility limit for an element is shared proportionally between the different isotopes of the same element. Sorption coefficient, diffusivity and porosity are given for each nuclide which allows cations and anions to be treated differently /SKB 2006a/.

The spatial discretisation used in the modelling of the KBS-3 system (the sub-division of the near-field into compartments) is described in a supporting document /Lindgren and Widén 1998/ where different discretisation techniques have been tested in order to find a discretisation that is course enough to allow for the problem to be solved using probabilistic calculations but yet fine enough allowing for the problem to be solved with acceptable accuracy. In order to be able to have a relative course spatial discretisation, analytical expressions are used at the mouth of the canister defect and at the fracture bentonite interface /Neretnieks 1986, Romero 1995, Kelly and Cliffe 2005/. The validity of the different models used in the code is discussed in the **Fuel and canister process report** and the **Buffer and backfill process report**.

In a dedicated test batch /Lindgren et al. 2006/, in the validity document, /Kelly and Cliffe 2005/ and in previous assessments, the capability in solving problems for the expected input data ranges has been shown. Input data for COMP23 is given through text files specified in the Proper documentation and the COMP23 user's guide. Based on the input files a system of differential equations is generated by COMP23 which is solved using the equation solver DASKR /Brown et al. 2005/. Compulink uses a subset of the COMP23 test batch /Vahlund and Hermansson 2006/.

3.8.3 Usage of the code

In the COMP23 user's manual /Romero et al. 1999, Cliffe and Kelly 2004/ the program and the models implemented are explained in detail. In addition to these documents, interactions between COMP23 and other codes and utility routines that is part of the Proper framework is described in the Proper documentation /Kjellberg 1999abc/. Text files are used to pass in-data and results to and from the code and the code is able to produce log-files in which it is possible to ensure that the right values have been used. For Compulink, /Vahlund and Hermansson 2006/ provides additional documentation.

3.8.4 Development process and verification

In a validity document /Kelly and Cliffe 2006/, the features of the code are presented and some of these are benchmarked against analytical solutions and in some cases to other codes. In addition to the validity document, a test batch /Lindgren et al. 2006, Vahlund and Hermansson 2006/ has been prepared in which the features of the code are demonstrated both for simple test cases which can be verified with analytical solutions or other codes and also for realistic KBS-3 cases using realistic data. Using the test batch the accuracy between different versions may be verified to ensure that code modifications does not change the capability of the code to solve the problem at hand.

In order to ensure functionality of the code on new machines, batch scripts are used to check out the current version from the version control system SCCS /Boghammar 1999/ (which is used for version control) and to set up the computational environment. Compulink uses subversion for version handling.

3.8.5 Rationales for using the code in SR-Can

The SR-Can team has selected the COMP23 and Compulink codes for the SR-Can safety assessment since it has been designed to solve the radionuclide transport problem at hand and since the knowledge of the code is good.

3.9 CONNECTFLOW

3.9.1 Introduction

CONNECTFLOW is the suite of Serco Assurance's groundwater modelling software /Serco Assurance 2005a/ that includes the NAMMU /Cliffe et al. 1998, Serco Assurance 2005d/ continuum porous medium (CPM) module and the NAPSAC /Serco Assurance 2005f/ discrete fracture network (DFN) module. CONNECTFLOW is also the name given to the concept of nesting CPM and DFN sub-models into a combined CPM/DFN model. A further module, GeoVisage, is a dedicated 3D visualisation application for interpreting the results from CONNECTFLOW. Hence, CONNECTFLOW is a very flexible tool for modelling groundwater flow and transport in both fractured and porous media on a variety of scales. NAMMU was originally developed as part of UK Nirex programme. NAPSAC was initially developed as part of the international Stripa project /Herbert et al. 1991, Herbert and Lanyon 1992/. Integration of the DFN and CPM concepts started as part of UK Nirex programme /Jackson et al. 1997/ and the Äspö Task Force /Holton and Milický 1997/. CONNECTFLOW is now maintained and developed through the international *iCONNECT* club /Holton et al. 2003/ (including SKB, Posiva, NAGRA and Obayashi) and by other commercial users. The simulations for SR-Can has been ran on a Linux cluster at Serco Assurance, Harwell UK. Due to the relatively large user base and the fact the code is of category 3 within SR-Can.

3.9.2 Suitability of the code

The fractured nature of the rocks in the Östhammar and Oskarshamn areas requires the consideration of both DFN and equivalent CPM models both to interpret the hydraulic properties of the rocks and to construct realistic models of flow and transport. CONNECTFLOW is unique in offering both these capabilities in the same package and allowing both approaches to be combined. In addition, CONNECTFLOW allows the modelling of a wide range of physical processes of relevance to SR-Can, such as: transient groundwater flow; saturated and unsaturated groundwater flow; coupled groundwater flow and salt transport; transport of reference water with rock matrix diffusion; coupled groundwater flow and heat transport; variable-density flow and transport in fracture networks; and radionuclide transport.

CONNECTFLOW has a long track-record of being used in the SKB programme since SR 97 /Boghammar et al. 1997, Hartley et al. 1998/. Bespoke developments have been made to suit the needs of site modelling and safety assessment calculations, /Marsic et al. 2001, Marsic et al. 2002/. The role of the software in the safety assessment was proposed in /SKB 2003/ and illustrated in the SR-Can interim assessment /Hartley et al. 2004, SKB 2004/. The use of CONNECTFLOW within SR-Can is a natural progression from its application in the site descriptive modelling exercises /Hartley et al. 2005ab/.

3.9.3 Usage of the code

The capabilities of CONNECTFLOW are described in the Technical Summary Document /Serco Assurance 2005a/. Input data is supplied to the code as text files and results are output as binary files and as an ASCII log-file which can be checked for errors, warnings and issues such as convergence. The syntax of the input and the input language is document in the HTML Command Reference Manual. The code can also be run using a Graphical User Interface (GUI) which is documented by an on-line User Manual. Checking of input files is recorded by the originator and then cross-checked by a second user.

3.9.4 Development process and verification

CONNECTFLOW is maintained and developed under an appropriate QA programme /Joyce 2005/ by the Environmental Management Department within Serco Assurance. The QA Programme conforms to the international standard BS EN ISO 9001 (1994) and to the TickIT Guidelines. The Concurrent Versions System (CVS) version management system is used to store all source code and test data for CONNECTFLOW. This automatically logs the author and date of each change to the system, and enables previous versions of the code to be accessed and recreated if necessary. All changes are thoroughly tested, and must be approved by the Software Manager before they are accepted. Through the CONNECTFLOW QA programme, Serco Assurance seeks to continually improve the quality and reliability of the program.

NAMMU has been verified within several international project including HYDROCOIN and INTRACOIN /SKI 1984, SKI 1986, NEA/SKI 1988/. NAPSAC was been verified within the STRIPA project /Herbert et al. 1991, Herbert and Lanyon 1992/. A full description of the verification of NAMMU and NAPSAC are given in /Serco Assurance 2005ce/. Testing of combined models is reported in the CONNECTFLOW Verification Manual /Serco Assurance 2005b/. Each release of CONNECTFLOW is verified by running a full test set for all modules of the software with well over 100 test cases.

3.9.5 Rationales for using the code in SR-Can

CONNECTFLOW is used in SR-Can for saturated groundwater flow calculation to provide groundwater flow and transport inputs to safety assessment calculations. Since the code allows alternative conceptual models, such as a DFN, it has some advantages over a purely porous medium approach. There are several experience users familiar with the SKB programme available to work on SR-Can.

3.10 Darcy Tools

3.10.1 Introduction

DarcyTools is a computer code for simulation of flow and transport in porous and/or fractured media. The fractured media in mind is a fractured rock and the porous media the soil cover on the top of the rock.

DarcyTools is a general code for this class of problems, but the analysis of a repository for nuclear waste is the main intended application.

A number of novel features are introduced in DarcyTools. The most fundamental is perhaps the method to generate grid properties (DarcyTools is a continuum porous-media code); a fracture network, with properties given to each fracture, is represented "directly" in the computational grid. This method is believed to result in very accurate anisotropy and connectivity properties. Another key feature is the grid system; an unstructured Cartesian grid which accurately represents objects, read into the code as CAD-files, is used in DarcyTools V3.0.

DarcyTools is developed through collaborative effort by SKB and CFE AB (Computer-aided Fluid Engineering AB) with CFE AB as the owner of the code. It builds upon earlier development of groundwater models, carried out by CFE AB during the last fifteen years. One such early development is represented by /Svensson 1991/, where predictions of inflows to the Äspö HRL, prior to its construction, are reported. At this time the general purpose equation solver PHOENICS /Spalding 1981/ was used. DarcyTools is based on the solver MIGAL /Ferry 2002/ and the development work on DarcyTools was initiated early 2001. The first well documented version of DarcyTools is v2.1, which was released in 2004. Version 3.0 is the version presently in use and the updated documentation of this version is scheduled for the spring of 2006. Both Windows XP and Red Hat Linux versions are available. The code is regarded as a category 4b code as the user base is small and limited to SKB projects.

3.10.2 Suitability of the code

Due to the collaborative (SKB and CFE AB) development of DarcyTools, it was from start decided that DarcyTools should be "the tailor-made SKB code". It is hence not surprising that the key features of the code match the requested capabilities in for example site investigations or glaciation studies. It is beyond the scope of the present text to describe these features (see Svensson et al. 2004a) but we may anyway mention: DFN-generation, free surface algorithm, multirate diffusion model and coupled groundwater flow and salt transport. In addition to useful features, a code needs to be efficient. The earlier mentioned unstructured grid in combination with the equation solver MIGAL (an unstructured multigrid solver) ensures that DarcyTools V3.0 is a state of the art code with respect to efficiency.

These features make DarcyTools V3.0 a suitable code for a wide range of problems that need to be considered by SKB.

3.10.3 Usage of the code

Three main documents /Svensson 2004, Svensson et al. 2004ab/ describe the code and its use in detail. Recent real world applications, for example /Follin et al. 2005/, provide another valuable source of information.

One of the documents is a User's Guide, which describe all input parameters. These input parameters make up the so called CIF (Compact Input File), which is written in XML format. DarcyTools also includes a Fortran input file, where more advanced features (transient boundary conditions, new source/sink terms, etc) can be introduced. Tecplot has been selected as the standard tool for post processing. Input files for Tecplot are readily generated.

An important part in the usage of the code is the monitoring of the simulation on the computer screen. Convergence parameters, development of variables in control points or profiles are plotted on the screen during the simulation. In V3.0 it is even possible to plot the distribution of variables in specified planes.

3.10.4 Development process and verification

One of the tree documents mentioned above /Svensson 2004/ deals with verification and validation. About thirty simple test cases, most with an analytical solution, are used to ensure that the equations are solved correctly. When a new major version of the code is released, all test cases are updated and checked to ensure both consistency with the old version and to make sure that the new version is correct. Validation is considered to be the process by which the code is shown to agree with measured data ("the right equations are solved"). A number of comparisons with field data are included in the above mentioned report. So far, no attempt to show that DarcyTools conforms to any international QA standard has been made.

3.10.5 Rationales for using the code in SR-Can

DarcyTools have been developed in cooperation with SKB especially for solving the problem at hand. The calculations have been performed with assistance by the developer of the code.

3.11 Eikos

3.11.1 Introduction

Eikos /Ekström and Broed 2006/ is a probabilistic engine which supports uncertainty and sensitivity analysis of models developed in Matlab and Simulink /The Mathworks Inc/. Eikos is fully integrated with Pandora used for nuclide migration calculations in the biosphere (Section 3.19). In SR-Can, Eikos was used to perform sensitivity analysis of ecosystem and landscape models developed in Pandora for the Forsmark and Laxemar sites. These models were used for derivation of the Landscape Dose conversion Factors (LDF) for SR-Can. Eikos was developed by Facilia AB and financed by Posiva OY and the Norwegian Radiation Protection Authority. The Eikos code is implemented as a toolbox in the commercial code Matlab and is regarded as a category 4a code.

3.11.2 Suitability of the code

The code Eikos includes state-of-the art sensitivity and uncertainty analysis methods, which can cope with linear, non-linear, as well as non-monotonic dependencies between inputs and outputs of the models. The following sensitivity analysis methods are supported by Eikos: Pearson product moment correlation coefficient (CC), Spearman Rank Correlation Coefficient (RCC), Partial (Rank) Correlation Coefficients (PCC), Standardized (Rank) Regression Coefficients (SRC), Sobol' method, Jansen's alternative, Extended Fourier Amplitude Sensitivity Test (EFAST), the classical FAST method, the Smirnov and the Cramér-von Mises tests. Eikos allows performing Monte Carlo simulations using simple random or Latin hypercube sampling.

3.11.3 Usage of the code

The Eikos user guide /Ekström and Broed 2006/ provide sufficient guidance for the use of the code and a full description of all implemented methods. As Eikos is fully integrated with Pandora, performing sensitivity and uncertainty analysis of models developed in Pandora is straightforward. The models developed in Pandora can be directly opened from Eikos and all parameters and simulation endpoints will be listed in the Eikos user interface. The users can then assign probability distributions or intervals to the parameters and perform the simulations.

3.11.4 Development process and verification

Eikos has been benchmarked, tested and compared with @Risk /Palisade Corporation/ which is a well established commercial code and with test functions that have exact analytical solutions /Ekström 2005/. These comparisons have shown that Eikos provides reliable results.

3.11.5 Rationales for using the code in SR-Can

The models used for biosphere modelling in SR-Can involve large number of parameters and complex relationships between the inputs and the outputs. The existing commercial tools, such as @Risk, support only the simplest sensitivity analysis methods, which do not perform optimally for these models. As Eikos is implemented in Matlab, it could be fully integrated with Pandora, which was the code used for biosphere modelling in SR-Can.

3.12 FARF31

3.12.1 Introduction

FARF31 /Lindgren et al. 2002/ is a Fortran 77 code used for radionuclide migration calculations in the far-field, i.e. the geosphere. It is based on a model with a one-dimensional advection-dispersion equation along a, possibly curved, stream tube coupled to a pure diffusion equation in the direction perpendicular to the centroid of the stream tube, for a number of radionuclides. Chain decay and ingrowth are included in the model. The concept of a stream tube can be compared to the combined effect of a large number of individual fractures all sharing the same inlet and outlet. The transversal dimension of the stream tube, the penetration depth, must be chosen by the user. The governing equations are solved in the Laplace domain using the groundwater travel time in the longitudinal direction as the independent variable to obtain a unit response function, which is subsequently convoluted with the input function to obtain the output function. The code was initially developed by SKB in the early 1990's as a submodel of the SKB safety assessment framework Proper. This framework is a collection of codes used for migration and consequence calculations through the near-field, the far-field and the biosphere, and uses standardised methods to transfer data and results between the different submodels. FARF31 has been used by SKB in the SR 95 /SKB 1995/, the SR 97 /SKB 1999/ and the SR-Can Interim assessments /SKB 2004/ of a final repository of the KBS-3 type. FARF31 has been continuously developed by SKB and subcontractors from its conception until the present version 1.2.1. Since the code has been developed by SKB, the code is belonging to category 4b.

3.12.2 Suitability of the code

The FARF31 code has been developed by SKB to be a reasonably accurate, simplified model of the fully three-dimensional far-field transport problem, which still is fast enough to allow for probabilistic calculations using the Proper package. The solution method, based on Laplace transformation of the governing equations and numerical inversion, limits its applicability to cases with constant transport properties, but this poses no problem at the present level of knowledge. However, a different solution method must be used to include colloid facilitated transport in the model (see the section about FARF33 below). Element specific porosity has recently been added to the model.

In a dedicated test batch (Appendix B in the FARF31 User's Guide /Lindgren et al. 2002/), in the validity document /Elert et al. 2004/ and in previous assessments, the capability of solving problems for the expected input data ranges has been shown. Input data for FARF31 is given though text files specified in the Proper documentation and the FARF31 User's Guide /Lindgren et al. 2002/.

3.12.3 Usage of the code

In the FARF31 User's Guide /Lindgren et al. 2002/ the program and its implementation and usage details are explained. An even more detailed description of the solution method can be found in /Norman and Kjellbert 1990/. In addition to these documents, interactions between FARF31 and other codes and utility routines that form the Proper framework are described in the Proper documentation /Kjellberg 1999abc/. Text files are used to pass input data to the code and results from the code. During each run log files are produced, which makes it possible to ensure the right parameter values have been used after the simulation has finished.

3.12.4 Development process and validation

In order to ensure the functionality of the code on new machines, batch scripts are used to check out the desired version from the version control system SCCS /Boghammar 1999/ and to set up the build environment. After every major code change resulting in a new version, the problems of the FARF31 test batch /Lindgren et al. 2002/ are used in regression tests of the code to ensure that its accuracy and reliability is intact.

3.12.5 Rationale for using the code in SR-Can

The SR-Can team has selected the FARF31 code for the SR-Can safety assessment since it has been designed to solve the radionuclide transport problem at hand and since the knowledge of the code is good.

3.13 FARF32

3.13.1 Introduction

FARF32 /Vahlund and Hermansson 2006a/ is a Fortran 77 code used for radionuclide migration calculations in a tunnel segment. It is based on a model with a one-dimensional advection-dispersion equation along the tunnel segment for a number of radionuclides. Chain decay and ingrowth are included in the model. The tunnel has one inlet and one outlet and a constant cross-section area. The concentration varies with time and the longitudinal coordinate but is assumed to be constant across any cross-section. The dependent variable is the sum of the concentration in both in a solute and a colloid phase. The governing equations are discretised in space using a first order finite volume scheme. The code has recently been developed by SKB as a submodel of the SKB safety assessment framework Proper. This framework is a collection of codes used for migration and consequence calculations through the near-field, the far-field and the biosphere, and uses standardised methods to transfer data and results between the different submodels. This will be the first time FARF32 is used in an assessment project. Since the code has been developed by SKB, the code is belonging to category 4b.

3.13.2 Suitability of the code

The FARF32 code has been developed by SKB to have a really fast implementation of the one-dimensional advection-dispersion equation compatible with the Proper system. The solution method of FARF32 is basically the same the one used in FARF33. It has been a goal to reuse existing code to the largest possible extent, and FARF32 and FARF33 shares all code but a few routines.

In the development report /Vahlund and Hermansson 2006a/ there is a section describing the validation work done so far. Input data for FARF32 is given though text files which, to a large extent, share the format with input files for FARF31 as specified in the Proper documentation and the FARF31 User's Guide /Lindgren et al. 2002/. A few differences related to the transport parameters and a few additions due the differences in the numerical solution method are only documented in the development report /Vahlund and Hermansson 2006a/.

3.13.3 Usage of the code

In the development report for FARF32 /Vahlund and Hermansson 2006a/ the program and its implementation and usage details are explained, and examples are given. In addition to this document, interactions between FARF32 and other codes and utility routines that form the Proper framework are described in the Proper documentation /Kjellberg 1999abc/. Text files are used to pass input data to the code and results from the code. During each run log files are produced, which makes it possible to ensure the right parameter values have been used after the simulation has finished.

3.13.4 Development process and validation

In order to ensure the functionality of the code on new machines, batch scripts are used to check out the desired version from the version control system SCCS /Boghammar 1999/ and to set up the build environment. After every major code change resulting in a new version, the intention is to use the problems of the FARF31 test batch /Lindgren et al. 2002/, possibly with some extensions, in regression tests also for FARF32 to ensure that its accuracy and reliability is intact.

3.13.5 Rationale for using the code in SR-Can

The SR-Can team has selected the FARF32 code for the SR-Can safety assessment since it has been designed to solve the radionuclide transport problem at hand and since the knowledge of the code is good

3.14 FARF33

3.14.1 Introduction

FARF33 /Vahlund and Hermansson 2006a/ is a Fortran 77 code used for radionuclide migration calculations in the far-field, i.e. the geosphere. Like FARF31, it is based on a model with a one-dimensional advection-dispersion equation along a, possibly curved, stream tube coupled to a pure diffusion equation in the direction perpendicular to the centroid of the stream tube, for a number of radionuclides. Chain decay and ingrowth are included in the model. The concept of a stream tube can be compared to the combined effect of a large number of individual fractures all sharing the same inlet and outlet. The transversal dimension of the stream tube, the penetration depth, must be chosen by the user. The main difference between FARF33 and FARF31 is that in FARF33 radionuclide transport can occur both in a solute and a colloid phase. There are constant coefficients for the rate of transfer between the phases in both directions. Filtering is taken into account by a constant ratio between the amount of mobile and immobile colloids. The governing equations are discretised in space using a first order finite volume scheme in both the longitudinal and the transversal direction. The code has recently been developed by SKB as a submodel of the SKB safety assessment framework Proper. This framework is a collection of codes used for migration and consequence calculations through the near-field, the far-field and the biosphere, and uses standardised methods to transfer data and results between the different submodels. This will be the first time FARF33 is used in an assessment project. Since the code has been developed by SKB, the code is belonging to category 4b.

3.14.2 Suitability of the code

The FARF33 code has been developed by SKB to in order to add the effects of colloid facilitated radionuclide transport to the well-known FARF31 model. The solution method of FARF31, based on Laplace transformation of the governing equations, could not easily be extended to this case, so a new code had to be developed. It has been a goal to keep the input data format compatible between FARF31 and FARF33, and to reuse existing code to the largest possible extent.

In the development report /Vahlund and Hermansson 2006a/ there is a section describing the validation work done so far. Input data for FARF33 is given though text files which share the format with input files for FARF31 as specified in the Proper documentation and the FARF31 User's Guide /Lindgren et al. 2002/. A few additions related to colloid transport and the different numerical solution method are only documented in the development report /Vahlund and Hermansson 2006a/.

3.14.3 Usage of the code

In the development report for FARF33 /Vahlund and Hermansson 2006a/ the program and its implementation and usage details are explained, and examples are given. In addition to this document, interactions between FARF33 and other codes and utility routines that form the Proper framework are described in the Proper documentation /Kjellberg 1999abc/. Text files are used to pass input data to the code and results from the code. During each run log files are produced, which makes it possible to ensure the right parameter values have been used after the simulation has finished.

3.14.4 Development process and validation

In order to ensure the functionality of the code on new machines, batch scripts are used to check out the desired version from the version control system SCCS /Boghammar 1999/ and to set up the build environment. After every major code change resulting in a new version, the intention is to use the problems of the FARF31 test batch /Lindgren et al. 2002/ in regression tests also for FARF33 to ensure that its accuracy and reliability is intact.

3.14.5 Rationale for using the code in SR-Can

The SR-Can team has selected the FARF33 code for the SR-Can safety assessment since it has been designed to solve the radionuclide transport problem at hand and since the knowledge of the code is good.

3.15 FracMan

3.15.1 Introduction

The FracMan software suite provides an integrated set of tools for discrete feature network (DFN) analysis of fractured and non-fractured heterogeneous rock masses. FracMan includes tools for discrete feature data analysis, geologic modelling, spatial analysis, visualization, flow and transport, and geomechanics. FracMan software is owned and distributed by the FracMan Technology Group of Golder Associates Inc.

The primary modules of FracMan are: FracSys (Data Analysis), FracWorks XP (3D DFN Structural Modelling and Visualization), MAFIC (Finite Element Flow and Transport Modelling). Several additional modules for network analysis and geomechanical analysis are available.

FracSys provides the tools to derive quantitative description of the geometry and properties of the discrete features from the types of data, which are typically collected as part of site characterization and exploration programs.

FracWorks XP is the core of the FracMan package, providing the discrete feature geological simulations, which form the basis for the discrete feature network (DFN) approach. FracWorks XP generates three-dimensional realizations of discrete feature geology using physically measurable parameters to produce geologically realistic discrete feature networks. DFN models created with FracWorks XP have been implemented for sites in sandstone, limestone/dolomite, siltstone, marl, and crystalline rocks. FracWorks XP also includes features for visualization, statistical analysis, simulated exploration, and simplified rock block, pathway, and network analysis.

MAFIC (Matrix and Fracture Interaction Code) uses the finite element method to solve for flow and transport through FracWorks XP geological models. MAFIC idealizes fractures using triangular finite elements, and provides a dual porosity interaction using either quadrahedral finite elements or a 1D approximation based on the Warren and Root pseudo-steady state approximation. MAFIC uses a pre-conditioned conjugate gradient solver, and has been applied for connected networks of up to 100,000 fractures.

3.15.2 Suitability of the code

The fractured nature of the rocks in the Forsmark and Simpevarp/Laxemar areas requires the consideration of DFN to interpret the geometrical behaviour of the fracture network. FracMan is a premier tool for analysing fracture network properties and developing geologically based models and has been pioneering the development of DFN codes since more than twenty years.

FracMan has a long track record in the nuclear waste programmes in Japan, France, Finland, Spain, USA and Sweden. The SKB programme has included FracMan studies in the Stripa project, at Äspö HRL and in the final site investigations. FracMan/MAFIC has been used extensively to interpret the hydraulic properties of the rocks and to construct realistic models of flow and transport. FracMan has also been used for assessing earthquake risks in Sweden and potential canister failure scenarios.

DFN models have developed in the site investigations in both the Forsmark and Oskarshamn Site descriptive model using FracMan.

3.15.3 Usage of the code

The usage of FracMan and the development methodology for establishing DFN models for the site investigations is described in detail for Laxemar in /Hermanson et al. 2005/ and for Forsmark in /La Pointe et al. 2005/. The general usage of FracMan is described in the user documentation by /Dershowitz et al. 1989/.

3.15.4 Development process and verification

FracMan software was developed specifically for radioactive waste management applications, with support from organizations including the US Department of Energy, Office of Crystalline Repository Development, and the Japan Atomic Energy Agency (JAEA, formerly PNC and JNC). FracMan software development is carried out within the Microsoft Source Safe Environment, which provides the following controls:

- All source code maintained and commented, including all versions back to 1990.
- Verification case input and output files and scripts to reproduce verification cases.
- Source code documentation and User Documentation.
- Logs of authors and explanations for each change and development to the software.

For the US radioactive waste management program, specific versions of the code are maintained used US Nuclear Regulatory Commission NQA-1 standards, within the US Department of Energy "Q" approval system, consistent with ISO-9001. For other radioactive waste management programs, specific software versions are tested against the US Department of Energy "Q" system version as required for specific applications.

FracMan software verification includes over 50 specific cases, which can be applied to ensure the accuracy of specific applications. Additional verification carried out for the International Stripa Project is described in /Dershowitz et al. 1989/.

3.15.5 Rationales for using the code in SR-Can

The FracMan code and its various add-ons was used for the construction of DFN models, that will be used within SR-Can. FracMan is not planned to be used in SR-Can for other purposes than to check the reported DFN models and produce representative realisations for communication purposes. However, FracMan might be used for computation of degree of utilisation but no such decision has yet been made.

3.16 Glacial isostatic adjustment software

3.16.1 Introduction

The GIA (Glacial Isostatic Adjustment) code is used to calculate the isostatic adjustment of the solid earth due to loading by ice and water during a glacial cycle. The gravitationally-consistent redistribution of water within the oceans is a central component of the algorithm, allowing accurate relative sea-level and shoreline migration to be predicted. In SR-Can the GIA code is used to reconstruct relative sea-level and shoreline positions in the regions of interest. It is also used to carry out sensitivity tests regarding e.g. the influence of earth and ice model parameters on the output.

The GIA code is a category 4b code, written in Fortran, and has been developed by Dr. G.A. Milne over a number of years in collaboration with Prof. J.X. Mitrovica at the University of Toronto /Milne 1998, Milne and Mitrovica 1998, Milne et al. 1999/. The complete version of the code, which includes all of the advances described below, is used by a small user base of postgraduate students and postdoctoral researchers working in either Milne's or Mitrovica's research groups.

The GIA code has been used in an extensive range of research projects. These include constraining mantle viscosities /Milne et al. 2001, Milne et al. 2004/, constraining former ice sheet volumes /Milne et al. 2002/, understanding Holocene sea-level change and modelling GIA effects around the world /Mitrovica and Milne 2002, Gehrels et al. 2004, Milne et al. 2005, Milne et al. 2006/, testing global melt scenarios /Clark et al. 2002, Bassett et al. 2005/, investigating the effect of 3D earth structure on GIA predictions /Whitehouse et al. 2006/, and identifying present-day melt sources and constraining the recent mass balance of polar ice sheets /Mitrovica et al. 2001, Tamisiea et al. 2001, 2003/.

3.16.2 Suitability of the code

The GIA code solves the sea-level equation /Farrell and Clark 1976/ via the pseudospectral approach developed by /Mitrovica and Peltier 1991/. The code has been significantly extended since this time to account for several different processes and thus improve the accuracy of the computation. Firstly, time-dependent shoreline positions are taken into account when calculating the ocean-loading function. Secondly, the water influx to regions vacated by retreating, marine-based ice is carefully accounted for in the distribution of the load /Milne et al. 1999/. And thirdly, changes to the rotational state of the Earth as a result of both surface and internal mass redistributions are considered. The theory that the most recent version of the code is based on and the algorithm employed to solve the governing equations are described in /Mitrovica and Milne 2003/ and /Kendall et al. 2005/. These publications define the state-of-the-art in computing sea-level changes associated with glaciation.

The code has a number of built-in analytical checks to ensure that the output is correct.

3.16.3 Usage of the code

Due to the nature of the development of the GIA code, and the intended user base, there is no formal documentation available.

The input data and parameters required by the GIA model are: 4D (spatial and temporal) global ice history for the duration of the model run; various radial Earth properties including the viscous properties of the Earth's mantle, the thickness of the Earth's lithosphere, elastic structure, density structure, and gravitational acceleration, as well as data relating to the shape of the Earth and its rotation (flattening coefficient and spin rate); and a global topography data set. The model was run over a range of time periods when carrying out the sensitivity tests, and time steps varied between 500 and 7,000 years, depending on the level of resolution required. Details of model setups and input data for individual SR-Can simulations are found in the **Climate report**.

At each time step, output data relating to relative sea-level, the height of the equilibrium sea surface, and solid earth deformation are calculated at each grid node. The computations are performed in the spherical harmonic domain at a truncation suitable for the region of study. For Fennoscandia, a truncation of 256 degree and order enables accurate predictions of relative sea-level and solid Earth deformation (vertical and horizontal). The model output is stored as an array of spherical harmonic coefficients and so predictions can be generated for any point on the surface of the Earth at each time step.

3.16.4 Development process and verification

In developing the code, a number of comparisons were made to analytical solutions wherever possible to test the accuracy of the numerical schemes employed.

A small number of research groups have developed their own sea-level code based on the results presented in the papers referenced above. However, not all versions include some of the latest developments discussed in the most recent papers (e.g. /Mitrovica and Milne 2003/). Some aspects of the software have been successfully benchmarked between various groups. However, a systematic benchmark between all groups based on the most recent version of the theory has not been completed.

For the SR-Can work it was necessary to determine shoreline positions within the Gulf of Bothnia during periods when the Gulf was cut off from the oceans, and a lake formed above sea level. The code was adapted to meet this specific requirement.

3.16.5 Rationales for using the code in SR-Can

The GIA code was used in SR-Can for simulating isostatic changes during the last glacial cycle for input to safety assessment calculations. The code was selected for the SR-Can safety assessment since it is one of the world-leading in its field.

3.17 Matlab and Simulink

3.17.1 Introduction

Matlab /The Mathworks Inc/ is a wide spread interactive environment and computing language for numeric computation, analysis and visual presentation. Matlab has been developed since the late 1970's and is globally wide spread. Matlab (in different versions) has been used for a variety of tasks in SR-Can for instance, migration calculations in all parts of the repository system (Sections 3.6, 3.9, 3.11 and 3.17) or when analysing fracture intersecting deposition holes, for pre- and post-processing of data or for visualisation tasks. The codes based on Matlab and uses the numeric solving capacity of the code or the graphical interface provided by Simulink, which is a platform for simulation and Model-Based Design of dynamic systems. Matlab and Simulink are clodesly related and are both products of Mathworks Inc.. While Matlab and Simulink on their own are regarded as a category 3 code, the advanced applications using Matlab are regarded as category 4 codes.

3.17.2 Suitability of the code

As Matlab and Simulink only provide the platform for different codes, the suitability is shown for each separate calculation task.

3.17.3 Usage of the code

Matlab and Simulink are both well documented codes and courses in using the codes are available.

3.17.4 Rationales for using the code in SR-Can

When performing numerical analysis tasks, Matlab and Simulink are one of few available codes and are well suited for their tasks.

3.18 MIKE SHE

3.18.1 Introduction

The near surface hydrological and hydrogeological code MIKE SHE (Système Hydrologique Europeen) is developed by the Danish Hydraulic Institute (DHI). The code describes all the different processes in the land phase of the hydrological cycle from rainfall to river flow. The model consists of five different compartments; saturated zone, unsaturated zone, overland flow, evapotranspiration and channel flow, Figure 3-1 in which the water flow is calculated in differently. In addition to the different compartments there is a frame component that takes care of the coupling and water exchange between the different compartments which runs simultaneously with the other components of the model. Transport calculations, particle tracking and advection-dispersion calculations, can also be performed within the MIKE SHE modelling tool.

MIKE SHE Version 2004b /DHI 2004/ has been used within the SR-Can modelling. The system is certified for Windows 2000 Professional and Windows XP Professional. The latest version of MIKE SHE, version 2005, is certified for Windows XP Professional X64 Edition. The code is commercial and is regarded as a category 3 code.

3.18.2 Suitability of the code

MIKE SHE is an advanced integrated hydrological system capable to simulate both surface and groundwater with the same precision as models focused on either groundwater or surface waters. The model is able to simulate the interaction between the surface water and the groundwater which is important when studying potential flow paths from the repository, i.e the water flow from the geosphere to the biosphere.

The precipitation can either be intercepted by leaves or fall to the ground. The water on the ground surface can infiltrate, evaporate or form overland flow. Once the water has infiltrated the soil, it enters the unsaturated zone. In the unsaturated zone, it can either be extracted by roots, and leave the system as transpiration, or it can percolate down to the saturated zone, see Figure 3-1. MIKE SHE is fully integrated with a channel-flow program, MIKE 11. When using the MIKE 11 code together with MIKE SHE, the two programs run simultaneously allowing for water exchange between the two codes during the whole simulation.

Based on the calculated flow field, particle tracking calculations (in the saturated zone) and advection-dispersion calculations can be performed. Within the SR-Can application both particle tracking and advection-dispersion calculations have been performed. The solute transport in the

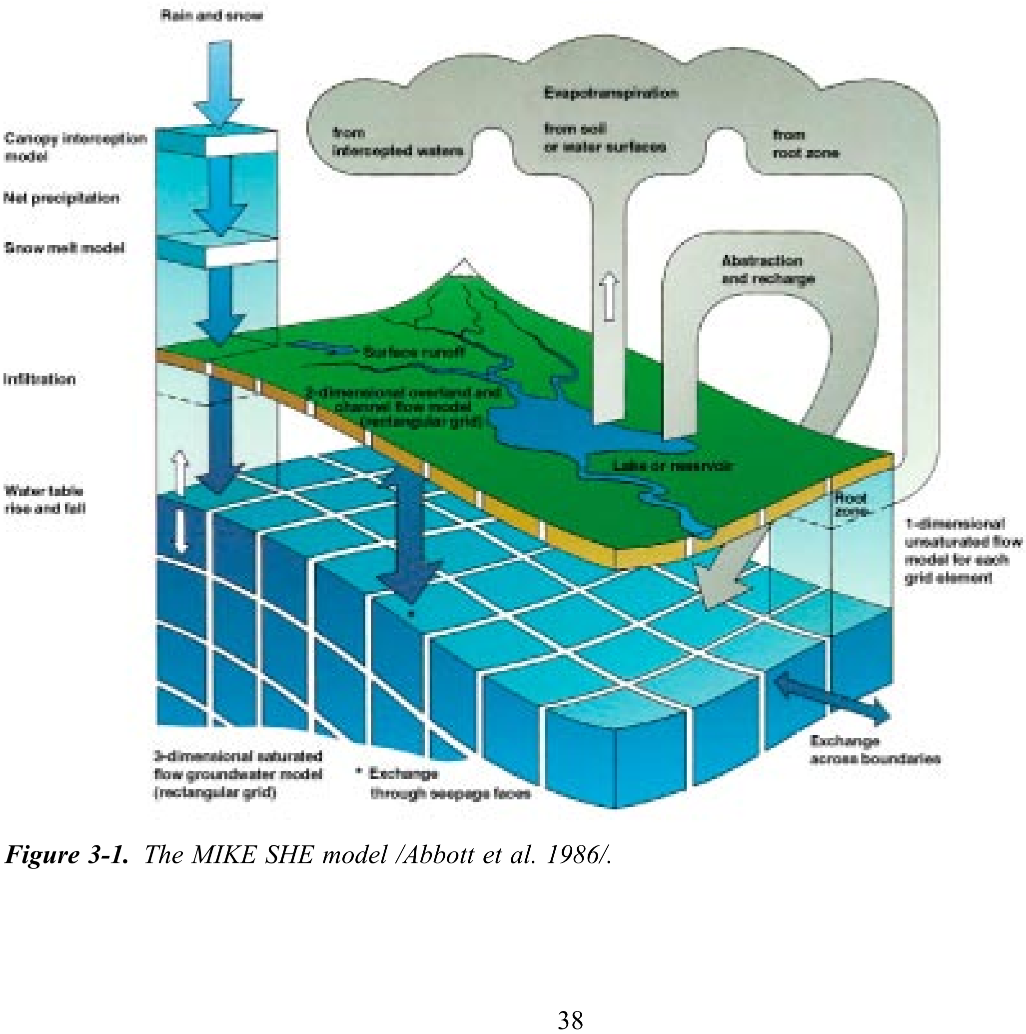

Figure 3-1. *The MIKE SHE model /Abbott et al. 1986/.*

advection-dispersion module can be calculated for all the components (overland, unsaturated zone and groundwater).

The following processes are included in the MIKE SHE advection-dispersion module:

- Water and solute transport in macro pores.
- Sorption of solutes described be either equilibrium sorption isotherms or kinetic sorption isotherms.
- Attenuation of solutes described by exponential decay.
- Plant uptake of solutes.

There is a direct coupling between MIKE SHE and the GIS program ArcMap which is part of the ArcGIS framework, see Section 3.4. This is a large advantage since most of the input data to the present modelling can be obtained in GIS format. It is possible to use both shape files and ESRI grid files as input. Both pre- and post processing can be made in the ArcGIS program.

3.18.3 Usage of the code

The MIKE SHE user manual /DHI 2004/ consists of three documents;

- Working with MIKE SHE:
  The document describes how to set up a model
- The MIKE SHE user reference:
  The document describes in detail the individual tools and dialogs the user is encountered to when working in the MIKE SHE user interface.
- The MIKE SHE Technical reference:
  The document includes detailed descriptions of the numeric engines used in the MIKE SHE modelling system:
  The different methods used in each component of the model are described in detail.

Input data is supplied to the code as text files, shape-files or ESRI-grid files. Result files are time series files, *.dfs0 or grid-files, *.dfs2. Both dfs0-files and dfs2-files are easily converted to text files. The dfs2-files can also directly be converted to GIS-format, shp-files or ESRI-grid files. An ASCII log-file is produced for each simulation, this file can be used to check for errors, warnings and issues such as convergence. The MIKE SHE model can also be run using a Graphical User Interface (GUI) which is documented by an on-line User Manual.

3.18.4 Development process and validation

The MIKE SHE model has it's origin in the SHE model, Systèm Hydrologique Européen, which became operational 1982. The model was developed by three organisations; the British institute of Hydrology, the French consulting company SOGREAH and the Danish hydraulic institute, DHI, which markets the MIKE SHE code today. The code is developed as new modelling ideas and needs are identified by the users. The latest version of the model is MIKE SHE version 2005.

The coupling between MIKE SHE and ArcGIS leads to a close integration with SKB's GIS-database. This ensures an acceptable level of quality as well as high level of traceability for the input data to the model.

Many organizations have reviewed and evaluated the MIKE SHE code. MIKE SHE has been selected as the best modeling tool for integrated groundwater/surface water modeling in many independent reviews, /e.g. Camp Dresser & McKee Inc 2001/. Each review has had different objectives and has used different criteria in the review process. A number of references is available at DHI website, (www.dhigroup.com).

3.18.5 Rationales for using the code in SR-Can

MIKE SHE is used in the SR-can for near surface hydrology and hydrogeology calculations. MIKE SHE makes it possible to model the integration between surface water, groundwater and evaporation processes and makes it possible to describe and understand the complexity of the water flows in the surface system.

3.19 Pandora

3.19.1 Introduction

The landscape models, used in the derivation of the Landscape Dose Factors for SR-Can, were implemented in the software package Pandora /Åstrand et al. 2005/. Pandora is an extension of the well-known codes Matlab and Simulink /The Mathworks Inc/. Pandora simplifies the development of compartment models consisting of large systems of ordinary differential equations and the handling of radionuclide decay chains. The Pandora tool comprises a library of Simulink blocks that facilitates the creation of compartment models and a standalone Toolbox for management of parameter values. The code has been developed by Facilia AB and financed by SKB and Posiva OY. The code is also used for biosphere modelling by Posiva OY. Since this code is an extension of commercial codes, it is regarded as a category 4a code.

3.19.2 Suitability of the code

Pandora was developed for the specific needs of the biosphere modelling required for the safety assessments of high level waste repositories. It has all required functionalities, including:

- handling of large sets of parameters,
- handling of time evolving parameters,
- representation of discrete transitions between states,
- handling of large number of radionuclides and decay chains,
- consideration of time evolving and spatially distributed discharges,
- Performing probabilistic simulations using the code Eikos (see Section 3.9).

Pandora extends the Simulink graphical user interface as to allow the user to easily inspect and modify the conceptual and mathematical models implemented.

3.19.3 Usage of the code

The Pandora code has a user guide /Åstrand et al. 2005/, which provides sufficient guidance for the additional functionalities that have incorporated to the commercial codes Matlab and Simulink. These codes are well documented and good support and updating is provided by the developers /The Mathworks Inc/.

The path to build a landscape model starts by creating a library of ecosystem models in Pandora, which facilitates handling several instances of the ecosystem models in the landscape model. For each landscape object, a Simulink subsystem is created, which includes models of all ecosystem types that may exist in the object during the whole simulation period. The discrete transition between ecosystem models is implemented using switches available in Simulink. The decay and in growth of radionuclides in a chain is handled with the help of the Pandora Radionuclide block.

For integrating the model, the user can choose from large list of solvers available in Simulink, including solvers that are appropriate for stiff systems of equations with discrete events. In SR-Can the solver ode15s was used. The activity concentrations and doses were calculated from the amounts of activity in different compartments predicted with the Pandora model by using a post-processing routine created in Matlab. Pandora is integrated with the code Eikos (see Section 3.11), which allows performing sensitivity and uncertainty analyses of the implemented models.

3.19.4 Development process and verification

Pandora has been benchmarked, tested and compared with other similar tools /Åstrand et al. 2005/. The solutions with the predecessor of Pandora (Tensit) were compared with analytical results, as well as with numerical results obtained with other simulation tools /Jones et al. 2004, 2005/. These comparisons have shown that Pandora provides reliable solutions.

3.19.5 Rationales for using the code in SR-Can

Pandora was contracted by SKB and Posiva OY for their specific needs in biosphere modelling. Both SKB and Posiva have been active in the development of the code, as to assure that the code satisfies all requirements, including quality assurance requirements. The decision to develop Pandora was taken after it was confirmed that other available commercial tools did not have all required functionalities.

3.20 Permafrost modelling code

3.20.1 Introduction

The code includes a mathematical expression for freezing and thawing of saline groundwater saturated bedrock. Originally, the code was used in the international project DECOVALEX III to investigate thermo-hydro-mechanical impacts of processes associated with freezing and thawing of subsurface during periods of glaciation/degalciation on the long term performance of a hypothetical post-closure repository /Hartikainen 2004, Chan et al. 2005/. In SR-Can, the code was used to perform a sensitivity analysis on the important factors and parameters affecting the development of permafrost and frozen ground, and to reconstruct the development of permafrost and frozen ground during the last glaciation cycle. The emphasis was on estimation of the maximum permafrost and frozen ground depths for relevant surface and subsurface conditions as well as for the presence of the initially heat-generating repository /SKB 2006b/. Recently, the code has been applied to estimate the development of permafrost and frozen ground at Olkiluoto, Finland for two future climate scenarios /Hartikainen 2006/.

The 2D finite element code was developed in the Laboratory of Structural Mechanics at the Helsinki University of Technology. Originally, the code was created for soil freezing problems /Hartikainen and Mikkola 1997, 2001, 2002, 2006/. The code is written in Fortran 77 and built on a general purpose finite element solver for non-linear non-stationary problems /Freund and Lempinen 1994/. The code is an open source code and is hence regarded as a category 3 code.

3.20.2 Suitability of the code

The permafrost model for freezing and thawing of saline groundwater saturated bedrock is based on the principles of continuum mechanics and macroscopic thermodynamics as well as on the theory of mixtures. The bedrock is considered as an elastic porous medium and the groundwater as an ideal solution of water and ionic solvents. The model describes heat transfer, freezing and melting of saline water, freezing induced cryogenic suction, groundwater flow and deformations of bedrock. Anisotropies of material properties such as permeability and thermal conductivity are allowed. From the code, the transportation of solutes, however, is excluded at the moment. A description of the model is given in /Hartikainen 2004/.

Information from ice-sheet modelling such as ice-sheet thickness, basal temperature and air temperature, as well as information from Global Isostatic Modelling regarding shoreline migration are given through boundary conditions.

The code based on the finite element method and implicit time integration schemes solves a set of coupled nonlinear partial differential equations, i.e. the energy balance, the mass balance of water and ice, and the equilibrium equations of internal and external forces, together with the state equations for water/ice phase change, groundwater flow and stress-strain relationships. A regularisation technique has been created to deal with discontinuities due to freezing, and the nonlinearities are solved by the Newton-Raphson method /Mikkola and Hartikainen 2002/.

3.20.3 Usage of the code

Description of the general finite element solver of the code is given in /Freund and Lempinen 1994/, and the computer implementation of the soil freezing model is presented in /Hartikainen 1994/. In the code, both input and output data as well as the runtime information of solution convergence and progress are dealt with in ASCII format. Matlab and GID, an interactive graphical user interface, are used to pre- and post-process the data.

3.20.4 Rationales for using the code in SR-Can

The code was used in SR-Can for simulating freezing of saturated bedrock in a number of sensitivity tests and in reconstructions of the last glacial cycle, all for input to safety assessment calculations. The code was selected for the SR-Can safety assessment since it is one of the world-leading in its field.

3.21 PHAST

3.21.1 Introduction

PHAST v.1 /Parkhurst et al. 2004/ simulates multi-component, reactive transport in 3D saturated groundwater flow systems. PHAST is a versatile groundwater flow and solute transport simulator with capabilities to model a wide range of equilibrium and kinetic geochemical reactions. The flow and the transport calculations are based on a modified version of HST3D /Kipp 1987, 1997/ that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with the geochemical code PHREEQC /Parkhurst and Appelo 1999/, which is imbedded in PHAST.

PHAST has been used in the SR-Can assessment for modelling different aspects of the near-field (canister and the engineered systems) behaviour.

The version of the code used has been updated as the authors release new versions in the web (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast/). The last version is PHAST v.1.2, but most of the work performed in the SR-Can has been carried out using the version v.1.

Since the code is an open source code, of a large user base and not written exclusively for the SR-Can project, the code is regarded as a category 3 code.

3.21.2 Suitability of the code

PHAST is a contrasted and robust geochemical code able to reproduce the different geochemical processes of interest in the SR-Can assessment.

The PHAST simulator is a general computer code with various reaction chemistry, equation-discretisation, boundary conditions, source-sink, and equation-solver options. Four types of flow and reactive transport simulations can be performed with PHAST: steady-state simulation of groundwater flow, transient simulation of groundwater flow, steady-state simulation of flow followed by reactive transport and transient simulation of flow with reactive transport.

PHAST solves a set of partial differential equations for flow and transport and a set of nonlinear algebraic and ordinary differential equations for chemistry. The equations that are solved numerically are the saturated groundwater flow equation for conservation of total fluid mass, a set of solute-transport equations for conservation of mass of each solute component of a chemical-reaction system and a set of chemical-reaction equations comprising mass balance equations, mass-action equations and kinetic-rate equations. The groundwater flow and solute-transport equations are coupled through the dependence of advective transport on the interstitial fluid-velocity field. The solute-transport equations and the chemical equations are coupled through the chemical concentrations terms. The chemical equations are fully coupled through the concentration terms and must be solved simultaneously.

By using a sequential solution approach for flow, transport and reaction calculations, numerical solutions are obtained for each of the dependent variables. Operator splitting is used to separate the solute-transport calculations from the chemical reactions calculations. Finite differences techniques are used for the spatial and temporal discretisation of the flow and transport equations.

More detailed information on the geochemical and transport equations solved can be obtained from the PHAST v.1 user's manual /Parkhurst et al. 2004/.

3.21.3 Usage of the code

In the PHAST v.1 user's manual /Parkhurst et al. 2004/ the program is explained in detail and a lot of examples are provided. In addition to this document the web page of the authors (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast/) also contains a lot of information and well documented examples as well as an active and interactive section of FAQ.

Reactive-transport simulations with PHAST require three input files: a flow and transport data file, a chemistry data file, and a thermodynamic data file. All data files are built with modular keyword data blocks. Each data block defines a specific kind of information (e.g. grid locations, boundary-conditions information, or initial chemical composition). All spatial data are defined by zones, which are rectangular volumes. All this information is easily introduced by means of .dat files.

Simulations results can be saved in a variety of file formats (ASCII or binary HDF). Results can be thus, easily post-processed by using the program PHASTHDF to extract subsets of the data stored in the HDF file and the program MODEL VIEWER (only for Windows) to produce 3D visualizations of the problem definition and of the simulation results. Both programs are distributed together with PHAST.

3.21.4 Rationales for using the code in SR-Can

The SR-Can team has selected the PHAST code for the SR-Can safety assessment since it is useful to solve 2D reactive transport problems in saturated zones. The knowledge of this program is high and good-supported.

3.22 PHREEQC

3.22.1 Introduction

PHREEQC v.2 /Parkhurst and Appelo 1999/ is a computer program written in the C programming language that is designed to perform a wide variety of low-temperature aqueous geochemical calculations.

It has been used in the near-field (canister and the engineered systems) in several ways. In some cases it has been directly used to perform simple 1D transport modelling but in most cases it has been used in the work realised previous to the use of the 2D transport modelling codes when studying the different geochemical systems considered.

The version of the code used is updated as the authors release new versions in the web (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/). Thelast version of the code is PHREEQC 2.12, but most of the work performed in the SR-Can has been carried out using the version 2.8, 2.9 and 2.10.

Since the code is an open source code, of a large user base and not written exclusively for the SR-Can project, the code is regarded as a category 3 code.

3.22.2 Suitability of the code

As the understanding of chemical behaviour of the near-field under different scenarios is of the main interest in the SR-Can, PHREEQC is the perfect tool to start with. It can be used as a speciation program to calculate saturation indices and the distribution of aqueous species (including redox elements). It is a good, robust and contrasted geochemical code.

PHREEQC is based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, exchangers and sorption surfaces, but also includes the capability to model kinetic reactions with rate equations that are completely specified in the form of Basic statements. It also includes a 1D algorithm that comprises dispersion, diffusion and various options for dual porosity media.

More detailed information on the geochemical and transport equations solved can be obtained from the PHREEQC v.2 user's manual /Parkhurst and Appelo 1999/.

3.22.3 Usage of the code

In the PHREEQC v.2 user's manual /Parkhurst and Appelo 1999/ the program is explained in detail and a lot of examples are provided. In addition to this document the web pages of both authors (http://www.xs4all.nl/~appt/a&p/ http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/) also contain a lot of information and well documented examples as well as an active and interactive section of FAQ.

Input data is easily introduced by means of the edit tool provided by the same program. Output data can be also easily selected and obtained in .txt or .dat files that can be read and modified with Microsoft Excel program or similar.

3.22.4 Rationales for using the code in SR-Can

The SR-Can team has selected the PHREEQC code for the SR-Can safety assessment since it is useful to characterize solutions (speciation, saturation-indexes) and make simple 1D dimensional transport calculations, as a previous step forward the use of bigger 2D codes. The knowledge of this program is high and good-supported.

3.23 RVS

3.23.1 Introduction

The Rock Visualization System (RVS) is a 3D CAD tool developed by SKB for use in visualizing geological and engineering data. It aims to assist in the interpretation of the geological environment by the construction of 3D structural geological models. These models supply a framework for the creation of integrated models covering all science areas, ultimately leading to the selection and design of the final repository system /Curtis et al. 2005/.

RVS has been under development since 1994. The current version of RVS, version 3.8, is based on MicroStation V8.5 and the database MS/Access 2000. The system is certified for Windows 2000 Professional and Windows XP Professional. Since the code has been developed by SKB, the code is regarded as a category 4a code. Updated versions of the program and descriptive reports will subsequently be released following further program development.

RVS has been developed for interpreting data collected during the Swedish radioactive waste disposal programme, including data from the Äspö Hard Rock Laboratory and from the potential disposal sites. Its focus is on the construction of structural geological models based on borehole and various forms of surface mapping data in crystalline rocks. Much of the necessary input to a model is in the form of primary data and the system has therefore been integrated with SKB's geological database SICADA. The acronym SICADA stands for SIte ChAracterization DAtabase, a relational database management system developed by SKB for the storage and maintenance of data collected during the site investigations. Models created in RVS can be exported in various formats for import and further analysis by other codes commonly used by SKB.

3.23.2 Suitability of the code

RVS has been developed as a Microstation application by SKB and is specifically tailored to SKB Project requirements with a code development that has been driven by Project needs.

RVS has been designed to enable a close integration with SKB's investigation database SICADA. Since all raw data originating from the many investigation programs is quality controlled before it enters SICADA, the close integration between the two systems ensures that this quality is maintained by automating data processing and transfer. This close integration ensures an acceptable level of data quality as well as ensuring a high level of traceability.

Work in native MicroStation is based on design files and levels, while work in RVS is object based. Drawing elements in a normal MicroStation design file have no intelligence in that they are simple graphical objects with specific graphical attributes that control their appearance. However, objects in an RVS-model often consist of a number of graphical elements, which together build a unit, linked to a local database with flexible tools for controlling their appearance. They are saved with a name in a logical structure depending on what they represent. All manipulative actions such as viewing selection and change of properties are done on the object level.

For the purposes of further external model development and analysis it is possible to save any model or a selection of objects as a standard Microstation design file, which in turn can be converted to a standard AutoCad drawing file. In addition to the proprietary *.rvs and *.dgn export formats, the geometry and parameter data of a model can be exported as an XML-file, which follows the rules laid down by W3C (The World-Wide Web Consortium). W3C's eXtensible Markup Language (XML) enables the creation of documents and databases whose contents are self-describing, i.e. the distinct items of data within such databases can be individually recognized and separately extracted from the medium in which they are typically stored and presented. The resulting export file format allows subsequent import to other visualization tools such as TechPlot and numerical modelling programs. This allows further science specific modelling and analysis work to be carried out on the geometrical framework representing the structural geological model created in RVS. The ultimate aim of this approach is to create an integrated geoscientific model covering the entire rock volume under study.

Since the development of RVS is driven by its users, modellers within various SKB-projects, the suitability for SKB needs is warranted. Various tailor-made add-ons to RVS have been produced to meet the needs of specific tasks.

3.23.3 Development process and validation

RVS has been under development since 1994. RVS version 3.8 is based on MicroStation V8.5 and the database MS/Access 2000. The system is certified for Windows 2000 Professional and Windows XP Professional.

The close integration with SKB's investigation database, SICADA, ensures an acceptable level of quality as well as high level of traceability for the input data to the model. RVS version 3.8 and SICADA have essentially the same structure to their parameter hierarchies. The request for data is made within RVS and then sent to SICADA via the Database Administration Server (DA Server). It is the DA Server, which accepts the order from RVS, interprets the request, searches the SICADA database, extracts and packages the required data and then sends the data parcel to the RVS user.

All of the visualizations and modelled objects, including the modelled structures, are defined as objects in RVS and appear in the Object Manager following an organized hierarchical tree structure. These object names are linked to their graphical representations in the design file by RVS as they are created.

SICADA is a dynamic database and some of the contained parameter data maybe subject to ongoing modifications and updates. In order to assist the user in keeping track of such changes and to ensure that the most up to date data is being used, RVS automatically notifies the user when existing parameter visualization is based on out of date values.

The modelling work involving RVS is carried out by a small team of individuals and a sequence of checks, reviews and reinterpretations is inbuilt into the model development process /see e.g. Munier et al. 2003/. Further, the models are checked by reviewers and members of a much larger project team before it is used for further analysis.

3.23.4 Rationales for using the code in SR-Can

RVS models constitute a de-facto standard for geological models within SKB. The choice of a commercial platform product, MicroStation, ensures reliable export/import of the models to a wide variety of formats. RVS models can host both the geometry of the modelled geological objects, 3D repository layouts and maps which makes it particularly suitable for a multidisciplinary working environment.

3.24 STATISTICA

3.24.1 Introduction

The commercial statistical software STATISTICA is an advanced data analysis package which provides a comprehensive array of data analysis, data management and data visualization procedures. Its techniques include a wide selection of predictive modelling, clustering, classification and exploratory techniques in one software platform. The STATISTICA 7.0 Base module, used by SKB, contains a comprehensive set of common statistical and visualisation tools in a user-friendly package. SKB also use the add-on products *STATISTICA Advanced*

Linear/Non-Linear Models, which contains a wide array of advanced modelling and forecasting tools, and *STATISTICA Multivariate Exploratory Techniques*, which offers a broad selection of multivariate exploratory techniques.

STATISTICA is a comprehensive statistical package which offers tools for almost all types of statistical analyses, as well as for a wide array of modelling tasks. It was developed by StatSoft from 1985 and onwards, and the first version of STATISTICA was released in 1991. STATISTICA was developed with Microsoft C/C++ compilers and other tools /StatSoft Inc 2001/. The product has today a wide-spread usage both in trade and industry, and in universities. StatSoft themselves estimate that STATISTICA has over 600,000 users worldwide (universities/research institutions: 30%; corporations/manufacturing facilities: 60%; government agencies: 10%) /StatSoft Inc 2005/. Due to the wide-spread use of the software, the code is classified in category 3 within SR-Can.

3.24.2 Suitability of the code

Because of its comprehensive array of statistical tools, STATISTICA is used by SKB as the main statistical software, both within SR-Can and in the site descriptive modelling. An extensive documentation of the product is available in the STATISTICA System Reference /StatSoft Inc 2001/, and there are also a number of basic and advanced statistics textbooks that use *STATISTICA* as their basis /StatSoft Inc 2005/.

3.24.3 Rationales for using the code in SR-Can

There is a need for an advanced data analysis package in SR-Can, both for statistical analyses and for modelling purposes. STATISTICA is one of the leading statistical packages on the market, with well documented success stories, and there are several experienced users of the programme in SKB.

3.25 Thermal model

3.25.1 Introduction

The purpose of this code is to calculate the temperature as a function of time in the repository as further described in /Hedin 2004/. The model builds on simple analytic expressions that produce similar results as numerical models, see further /Hedin 2004/. The model is implemented in Microsoft Excel by the user. No rigorous version control system has been applied during the development of the code.

An earlier version of the code was used in the SR-Can Interim report /SKB 2004/. No changes of the model implementation have been made to that version.

Since the code has been developed by SKB, it is of category 4b.

3.25.2 Suitability of the code

The capability of the code to correctly solve the problem is documented in /Hedin 2004/ where benchmark exercises to numerical and similar analytic models are described. The code consists of analytic expressions that are directly evaluated in Microsoft Excel and a table of pre-calculated numerical integrals.

The parameter ranges used in the benchmark exercises are similar to those used in SR-Can. Since the benchmark exercises show good agreement, it is concluded that the code fulfils its purposes.

3.25.3 Usage of the code

A simple manual has been produced for the analytic model, available in the SR-Can project archive. The code has been used mainly by the implementer. The Excel spreadsheets should be self-explanatory for an external user, together with the model description in /Hedin 2004/ and the manual.

Input data are entered in the Excel spreadsheets as an integrated part of the code. Input and output data are obtained directly in the spreadsheet. The code may be run probabilistically using the Excel plug-in @Risk /Palisade corporation/. A comprehensive manual is available for the latter.

3.25.4 Development process and verification

The code consists of analytic expressions directly evaluated in Microsoft Excel, for which verification of the correctness of the mathematical solution is provided by the developer of Excel.

Consistency of results between different versions is not yet an issue since the first version of the code is used in SR-Can.

3.25.5 Rationales for using the code in SR-Can

The SR-Can team has selected the thermal model to be used in the safety assessment since it produces similar results as more complex codes, since it is fast and directly available for use by the SR-Can team.

3.26 UMISM

In SR-Can the UMISM code was used to reconstruct the Weichselian ice sheet during the last glacial cycle, and for a number on sensitivity test regarding e.g. maximum ice sheet thickness. UMISM (University of Maine Ice Sheet Model) is a dynamic ice-sheet model capable of simulating realistic ice sheets that are typically not in balance with climate (advancing/retreating).

3.26.1 Introduction

The climate input, forcing ice sheet evolution, is the mean annual air temperature at sea level, and its variation over time. The mass balance is determined from an empirical relationship constituting a simple parameterisation of the ice sheet's effect on local climate /Fastook and Prentice 1994/. Distributed air temperatures over the model domain are determined from height over sea level and distance from the pole. The UMISM model includes a mathematical description of precipitation from a number of other parameters; distance from the pole, saturation vapour pressure (function of altitude and laps-rate), and surface slope. This is an empirical relationship developed from the Antarctic ice sheet /Fastook and Prentice 1994/. Over a certain model domain, with a topography described from a Digital Elevation Model (DEM), this climate description gives a spatial pattern of air temperatures at ground level and a pattern of precipitation. Given a suitable climate forcing, the model develops a thermo-dynamic ice sheet over the DEM. Derived ice temperatures, together with density variations with depth, control ice hardness and ice flow. The thermodynamic calculation accounts for vertical diffusion, vertical advection, and heating caused by internal shear.

The UMISM ice sheet model includes a simplified isostatic description for the deformation of the crust due to the weight of the modelled ice sheet configuration. The UMISM code also includes a high-resolution modelling option by nesting.

The UMISM finite-element code (Fortran) has been developed by Prof. J. Fastook, at Computer Science dept. at Univ. of Maine, U.S., over an extended period /e.g. Fastook and Chapman 1989, Fastook 1990, Fastook 1994, Fastook and Holmlund 1994, Fastook and Prentice 1994, Johnson 1994/.

In the ice sheet reconstruction simulations, inputs parameters to the model were: landscape topography, geothermal heat flux, global sea-level variations, thermo-mechanical properties of the ice, isostatic properties of the Earth's crust, and annual air temperature at sea level. In these simulations the code was run for 120,000 years with 5 year time steps. For each time step, output data were calculated for each grid cell and grid node, data such as: ice thickness, englacial and basal ice temperatures, ice velocity, direction of ice movement, isostatic depression of crust, and amount of basal melting or freeze-on of water.

Output data from UMISM can be saved in NetCDF (Network Common Data Form a standard data format).

3.26.2 Suitability of the code

UMISM was part of the EISMINT (European Ice Sheet Modelling Initiative) model intercomparison experiment and yielded output in agreement with many other major ice sheet models /Huybrechts et al. 1996, Payne et al. 2000/.

The UMISM has previously been used for a large number of simulations of Fennoscandian ice sheets for various purposes /cf Fastook and Holmlund 1994, Holmlund and Fastook 1995, Näslund et al. 2003/.

3.26.3 Usage of the code

Descriptions of model setups, as well as input data to the model, for SR-Can simulations are found in the **Climate report**.

3.26.4 Development process and verification

The code was adapted to meet specific requirements during the SR-Can work, for instance to produce certain type of output data related to the production of glacial melt water. Specific output data formats were also produced for data export to other SR-Can projects, such as the ground-water flow modelling by Colenco, permafrost modelling conducted at the Technical university of Helsinki by J. Hartikainen, Global Isostatic Modelling conducted at University of Durham by P. Whitehouse and G. Milne, and for modelling of crustal stresses performed at university of Uppsala performed by B. Lund.

3.26.5 Rationales for using the code in SR-Can

UMISM is used in SR-Can for simulating the behaviour of the dynamic behaviour of the ice sheet during the last glacial cycle for input to safety assessment calculations, and also for input to simulations of other phenomena such as permafrost, isostatic changes, crustal stress, and ground water flow.

The UMISM code was selected for the SR-Can safety assessment since a very large number of simulations of the Fennoscandian ice sheet have been done with the UMISM model over the years. One major benefit from this is that it has provided a big experience of how to do model calibrations against geological observations in order to obtain more realistic ice sheet configurations. An additional reason for choosing this model in the safety assessment is the recognized ability and interest of the model developer to engage in validating and assessing model results against real-world observations and phenomena related to the ice sheet system that is being modelled. This is important in phases of model calibration as well as when adopting and developing the model to specific needs of the project.

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Appendix A

Assessment model flowcharts, AMFs

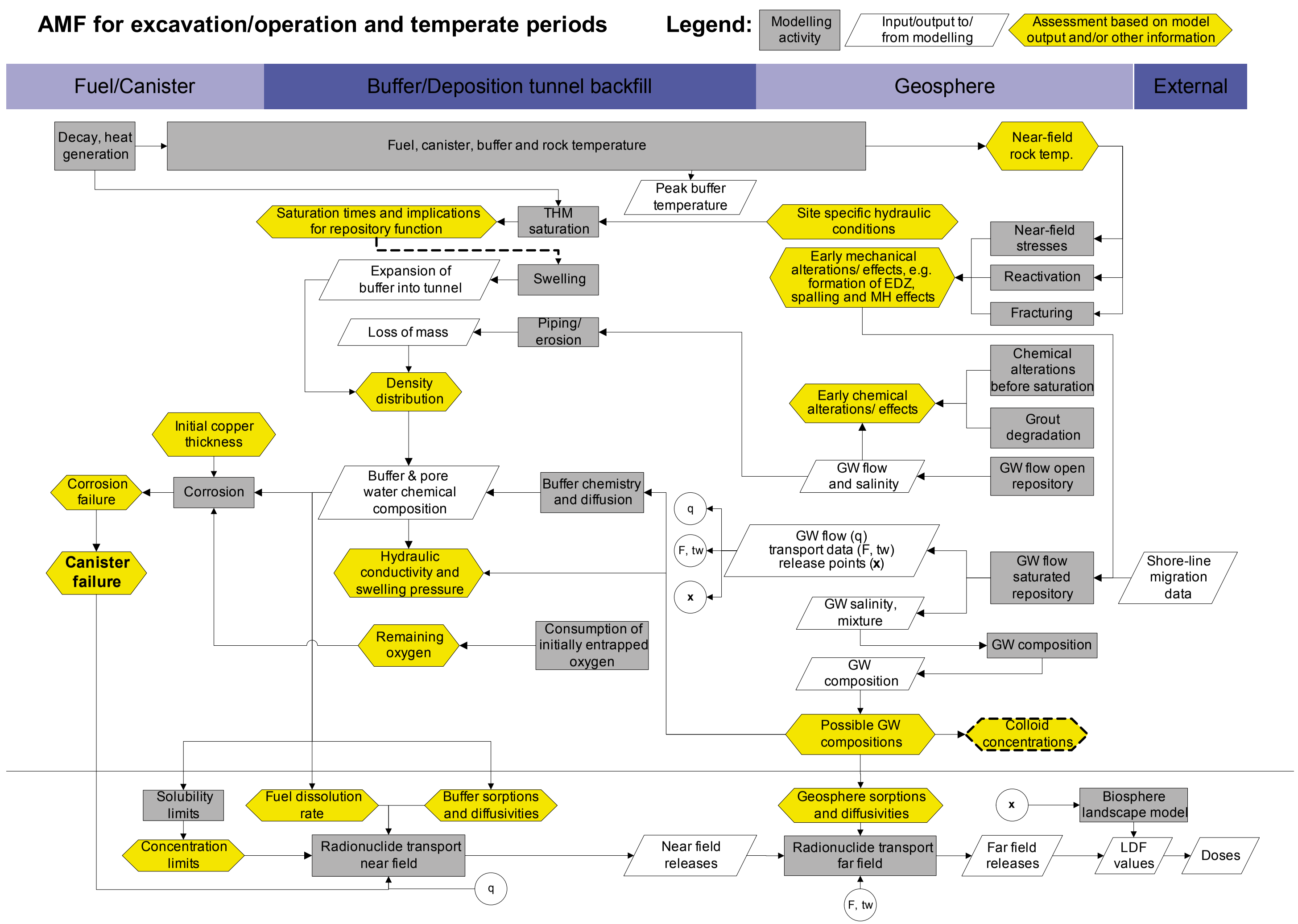

Figure A-1. Assessment model flow chart for the excavation/operation period and the initial temperate period after closure.

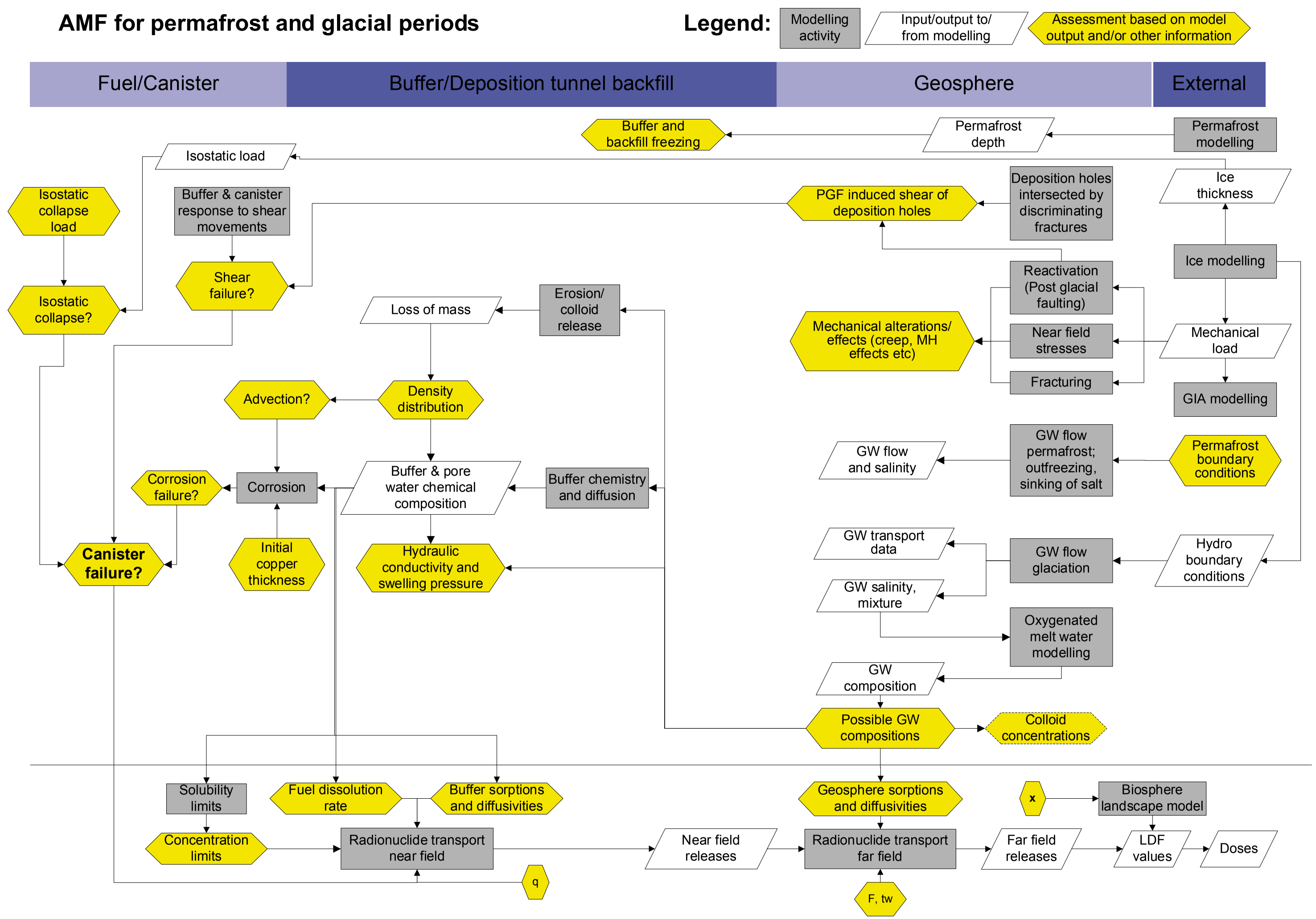

Figure A-2. Assessment model flow chart for permafrost and glacial conditions.

Appendix B

Presentation of the codes

Table B-1. Codes used for modelling activities presented in the AMF for the excavation/operation and temperate periods.

Modelling activity in AMF	Code	Code presented in section
Decay, heat generation	Scale 4–3, ORIGEN-S, CASMO 4[1]	
Near-field temperature	Ansys, Analytical model (Excel)	3.5
THM Saturation (buffer and backfill)	ABAQUS	3.2
Near-field stresses (geosphere)	3DEC	3.1
Reactivation	3DEC	3.1
Fracturing (spalling)	3DEC	3.1
Chemical alterations before saturation (geosphere)	PHAST	3.21
Grout degradation	PHAST	3.21
Groundwater flow open repository	DarcyTools	3.10
Groundwater flow saturated repository	ConnectFlow	3.9
Groundwater chemistry	PhreeqC	3.22
Piping/erosion	Simple scoping calculation[2]	
Swelling	ABACUS, CodeBright	3.2, 3.7
Buffer chemistry and diffusion	PHAST	3.21
Consumption of initially entrapped oxygen (buffer and backfill)	PHAST	3.21
Corrosion	Analytical expressions (Excel)[2]	
Concentration limits	PhreeqC	3.22
Radionuclide transport near-field	COMP23/Compulink, Analytic model (Excel)	3.8
Radionuclide transport far-field	FARF31, Analytic model (Excel)	3.12
Biosphere landscape model	Eikos, MIKE SHE, Pandora and Statistica	3.11, 3.18, 3.19, 3.24

1. Calculations performed prior to SR-Can reported in /Håkansson 2000/.
2. Category 2 code, not covered.

Table B-2. Codes used for modelling activities presented in the AMF for permafrost and glacial periods.

Modelling activity in AMF	Code	Reported in section
Permafrost modelling	Numerical permafrost model	3.20
Ice modelling	UMISM	3.26
GIA modelling	Numerical GIA model	3.16
Deposition holes intersected by discriminating fractures	Matlab, Analytical expressions (Excel)	Matlab
Near-field stresses (geosphere)	3DEC	3.1
Reactivation	3DEC	3.1
Fracturing	3DEC	3.1
GW flow permafrost; outfreezing, sinking of salt	DarcyTools	3.10
Groundwater flow, glaciation	ConnectFlow	3.9
Oxygenated melt water modelling	PhreeqC	3.22
Erosion/colloid release	Analytical expression[1]	
Buffer chemistry and diffusion	PHAST	3.21
Buffer and canister response to shear movements	ABAQUS	3.2
Corrosion	Analytical expressions (Excel)[1]	
Solubility limits	PhreeqC	3.22
Radionuclide transport near-field	COMP23/Compulink, Analytic model (Excel)	3.8
Radionuclide transport far-field	FARF31, FVFARF, Analytic model (Excel)	3.12, 3.13
Biosphere landscape modell	Eikos, MIKE SHE, Pandora and Statistica	3.11, 3.18, 3.19, 3.24

1. Category 2 code, not covered.

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