R-08-17

Model summary report for the safety assessment SFR 1 SAR-08

Svensk Kärnbränslehantering AB

March 2008

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 250, SE-101 24 Stockholm
Tel +46 8 459 84 00

ISSN 1402-3091
SKB Rapport R-08-17

Model summary report for the safety assessment SFR 1 SAR-08

Svensk Kärnbränslehantering AB

March 2008

Keywords: dokID 1095366.

Preface

This document is the model summary report for the safety assessment SFR 1 SAR-08. In the report, the quality assurance measures conducted for the assessment codes are presented together with the chosen methodology. The document constitutes one of the references used in the safety analysis SFR 1 SAR-08.

Anna Gordon, SKB has compiled the report.

This document has been reviewed and all comments have been documented in accordance with SKIFS 2004:1.

Stockholm, February 2008

Anna Gordon

Project leader, SFR 1 SAR-08

Summary

This document is the model summary report for the safety assessment SFR 1 SAR-08. In the report, the quality assurance measures conducted for the assessment codes are presented together with the chosen methodology.

In the safety assessment SFR1 SAR-08, a number of different computer codes are used. In order to better understand how these codes are related an Assessment Model Flowchart, AMF, has been produced within the project. From the AMF, it is possible to identify the different modelling tasks and consequently also the different computer codes used. A number of different computer codes are used in the assessment of which some are commercial while others are developed for assessment projects. 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

This document constitutes a reference to the SFR 1 SAR-08 safety assessment. In the following, the objectives, scope and structure of this document is presented.

1.1 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 SFR 1 SAR-08 and the quality assurance procedures and documents relating to the codes. More specifically, the report contains

- Assessment model flow chart (AMF) that describes the modelling tasks in SFR 1 SAR-08 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, data transfer between models, QA measures for code development, version control, etc.

The aim is however not to present reasons for including a certain process in the modelling or to justify the selected input data.

1.2 Structure of the report

In the current chapter, the purpose of the report 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, an assessment model flowchart, AMF, is initially introduced in which the different calculation tasks performed in the assessment can be identified. While some of the quantification tasks identified in the AMF are simple scoping calculations other require more 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. In Table 1-1 each modelling activity in the AMF is coupled to the code used for that specific task and a section in this report where the code is presented.

Table 1-1. Codes used for modelling activities in SFR 1 SAR-08 presented in the AMF.

Modelling activity in AMF	Code	Code presented in section
Biosphere landscape model	Pandora Eikos	3.6 3.3
Climate dependent hydrology model	DarcyTools	3.2
Degradation of EBS	PhreeqC	3.8
Geosphere hydrology	Geoan	3.4
GIA model	Glacial isostatic adjustment software	3.5
Ice sheet model	UMISM	3.9
Permafrost model	Permafrost modelling code	3.7
Radionuclide transport far field	Amber	3.1
Radionuclide transport near field	Amber	3.1
Regional hydrology	Geoan	3.4
Repository hydrology	Geoan	3.4

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 SFR 1 SAR-08 is described. To do this, an assessment model flow chart, AMF which provide an overview of all major models and the flow of information between them are initially presented. From the AMF, 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 Assessment model flow chart

To illustrate how major modelling tasks in the assessment are related, an assessment model flow chart, AMF, has been constructed for SFR 1 SAR-08, see Figure 2-1. In the AMF, 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 (repository, geosphere and external). Additional input data, coming from other sources than the models presented in this report, are not included in the AMF.

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.

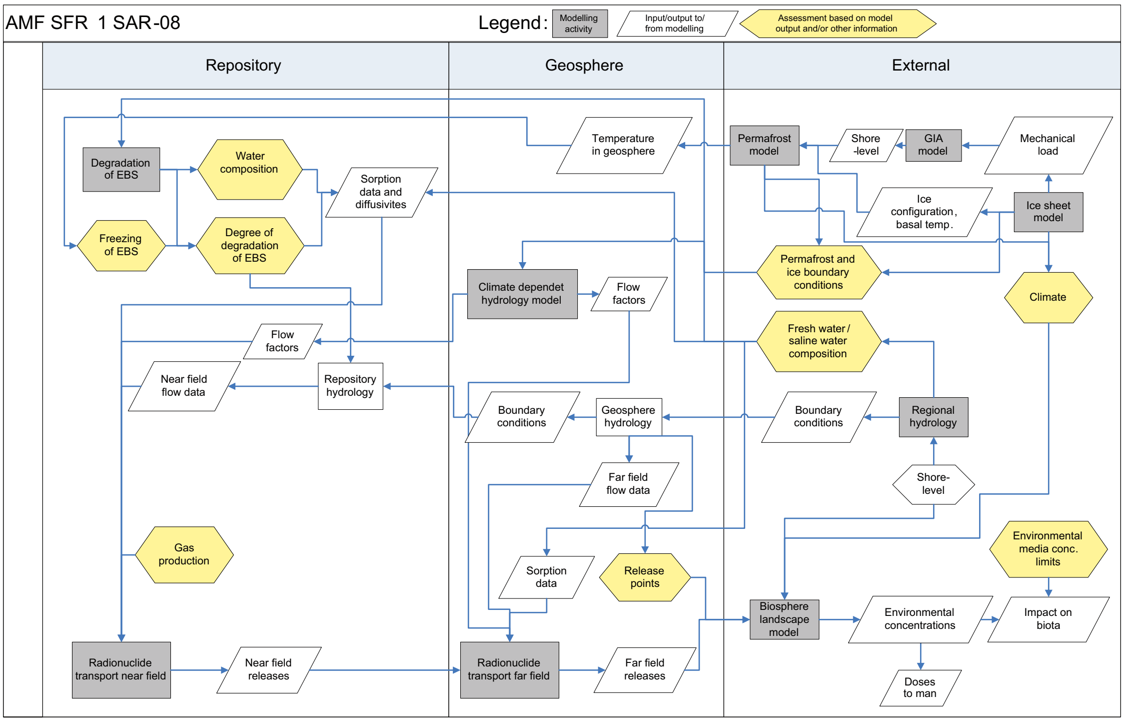

Figure 2-1. Assessment model flow chart for SFR 1 SAR-08

2.2 Types of codes used in the assessment

As seen in for instance the SR-Can main report /SKB 2006a/ a large number of different computer codes are commonly used when performing a safety assessment. The complexity of assessment codes may range 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 may 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 assessment. For codes developed within the assessment project, the source codes are available for external review. For the commercial codes this is normally 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 assessment is limited. Codes in this category are not written exclusively for the assessment 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. 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 the assessment 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 the assessment.

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 Table 1-1, 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 right requirements exist for the code to be 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 SFR 1 SAR-08 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 SFR 1 SAR-08 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 SFR 1 SAR-08 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 both by the user and by the code.

This part may be written either by the SFR 1 SAR-08 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 and used in SFR 1 SAR-08 (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 SFR 1 SAR-08 team or by subcontractors using the code.

2.4.5 Passing data between models

In this section it is described how data are passed between the model that is described and other models identified in the AMF. The difference between how handling of data is described in this section and in the section "Usage of the code" is that the current section deals with data passed between different models while the former handles data handling internally.

2.4.6 Rationales for using the code in SFR 1 SAR-08

Under this heading, the formal decision by the SFR 1 SAR-08 team to use the code in the assessment is presented together with a brief motivation, this text is written by the SFR 1 SAR-08 team.

3 Description of the codes

This chapter provides a listing of the codes used in the SFR 1 SAR-08 safety assessment based on the models identified in the assessment model flowcharts. Each code and it's associated model are presented in Figure 2-1. The text for each code follows the outline presented in Section 2.3.

3.1 Amber

3.1.1 Introduction

AMBER, a commercially available compartment modelling code which runs on Windows desk top computers, is a general-purpose tool. It allows the development of compartment models, and calculation of their solutions, for a wide range of situations. AMBER is a linear donor controlled compartment class of model and it can be applied to a very wide range of problems as a result of the flexibility with which transfers between compartments can be specified. Documentation of AMBER /Enviros and Quintessa 2006a/ and its use are provided by Enviros, the owners of AMBER.

Although the models that can be set up in AMBER are limited to those of the donor controlled compartment type, this class of models can be applied to a very wide range of problems as a result of the flexibility with which transfers between compartments can be specified. AMBER has been applied to a wide range of problems concerned with the way that radionuclides and other contaminants move through different parts of the environment including safety and performance assessment.

Prior to the near- and far field radionuclide transport calculations for SFR 1 SAR-08 /Thomson et al. 2007b/ an intercomparison study with the corresponding calculations performed for the SAFE project were successfully conducted using AMBER version 5 /Thomson et al. 2007a/. AMBER has been used in for previous performance assessments for SKB by Enviros /Thomson and Miller 2005/.

3.1.2 Suitability of the code

AMBER is not a specific defined model but a modelling code that enables the user to develop a conceptual model to meet their specification, consequently AMBER has been applied in many projects. The AMBER Users and References document /Enviros and Quintessa 2006b/ includes a list of publications that describe assessments in which AMBER has been applied. The proven application of AMBER to a variety of projects is the best way of demonstrating the suitability of the code.

AMBER was successfully used in the Vault Test Case of the IAEA's ISAM programme to model the migration and fate of liquid and solid releases from a near-surface radioactive waste repository /IAEA 2003a/. The results obtained from AMBER were in agreement with those obtained using other internationally recognised codes.

AMBER was used in support of the IAEA's BIOMASS programme /IAEA 2003b/. The results for Example Reference Biospheres (ERBs) 2A and 2B were obtained following their implementation in AMBER. Very close agreement was achieved when the AMBER results for ERB 2A were compared with the results achieved following its implementation in a different software package.

The performance of AMBER was evaluated against the Pacific Northwest Laboratory's MEPAS code and Andra's AQUABIOS code in assessing the environmental impact of non-radioactive contaminants /Côme et al. 2004, ANDRA 2003/. The project demonstrated close agreement between AMBER and the other codes.

AMBER models, in conjunction with models from IPSN and ANDRA (France) have been used in an IAEA study to derive activity limits for the near-surface disposal of radioactive waste /IAEA 2003c/.

Models developed using AMBER have been compared against other models in BIOMOVS II. QuantiSci (now Enviros Consulting Limited) developed an AMBER model for the C-14 release to a lake scenario /BIOMOVS II 1996a/, whilst Ciemat (Spain) developed models for the Complementary Studies /BIOMOVS II 1996b/ and lysimeter /BIOMOVS II 1996c/ exercises.

In an application to subsurface transport, AMBER models have also been used by an MSc student to represent the migration of contaminants in an aquifer and the results successfully compared against analytical solutions /Scott 1998/.

The validity of the equations for solving radionuclide transport in a system of backfilled compartments is discussed in the SR-Can Buffer and Backfill process report /SKB 2006b/ and in the COMP23 validity document /Kelly and Cliffe 2006/. For the geosphere, the validity of using the advection – dispersion equation with matrix diffusion in the transverse direction is discussed in the SR-Can Geosphere process report /SKB 2006c/. The implementation in a compartment based code is however slightly different than that used in the semi-analytical FARF31 code which was used in SR-Can. Using a compartment based approach for solving this problem has however been done in several other assessment calculations for instance /Maul et al. 2003/ and /Enviros and Quintessa 2005/.

The mathematical implementation in AMBER makes it suitable for solving problems where long time frames are analysed, such as the problem at hand.

3.1.3 Usage of the code

The general documentation available for AMBER is extensive /Enviros and Quintessa 2006abcd/.

More specifically the implementation of Project SAFE in AMBER /Thomson et al. 2007a/ is described providing a comprehensive breakdown of the model where AMBER has been used to undertake assessment calculations on all of the disposal system, including all disposal tunnels and the Silo, the geosphere and several biosphere modules.

In undertaking the comparison of AMBER with the various codes and calculation tools used in Project SAFE /Thomson et al. 2007a/ it was necessary to undertake a detailed analysis of the modelling approach previously adopted, with particular focus given to the near-field models. As a result some discrepancies in the implementation of the models and documentation were noted.

The exercise demonstrates that AMBER is fully capable of representing the features of the SFR 1 disposal system in a safety assessment. Additional information on the usage of the code, as well as the results are provided /Thomson et al. 2007b/ by Enviros.

3.1.4 Development process and validation

AMBER is developed by Enviros Consulting Limited and Quintessa Limited. Additional technical and/or financial assistance has been provided by Centro de Investigaciones Energéticas Medioambientales y Tecnológicas (CIEMAT), Universidad Politecnica de Madrid (UPM), Empresa Nacional de Resíduos Radiactivos S A (ENRESA), JGC Corporation, the Japan Atomic Energy Agency (JAEA), the Swedish Nuclear Power Inspectorate (SKI), the United Kingdom Atomic Energy Authority (UKAEA) and UK Nirex Limited.

In the verification report /Robinson 2008/ indicate a number of tests that have been successfully completed to demonstrate the stated functionality of AMBER is achieved. Importantly, that due to the nature of the AMBER's code, the verification report presents validation of the underlying mathematical basis for the code proving that the models are solved correctly in accordance with what has been specified. The verification of the models themselves, as opposed to the computer code, is the responsibility of the model developer who uses AMBER.

AMBER has been used in the development of the performance assessment of SFR 1 SAR-08. As part of SKI's review of SKB's calculations for the SFR 1 repository for low and intermediate level waste, AMBER was used to undertake an exploration of some of the important issues /Maul and Robinson 2002/. As well as demonstrating the applicability of AMBER in an overall performance assessment, the calculations include direct comparisons with SKB calculations. Given the slightly different modelling assumptions made, the results agree well.

In addition, SKI and SSI have undertaken an intercomparison between AMBER and Ecolego to give confidence in their application to total-system performance assessment (PA) studies for deep repositories and to further review SKB's SR 97 calculations /Maul et al. 2003, 2004/. The studies compared the results for near-field, geosphere and biosphere implementations, considering both deterministic and probabilistic calculations. The studies demonstrated good agreement between the two codes.

SKB have used AMBER as the benchmark against which to tested their Tensit simulation tool /Jones et al. 2004/. The study demonstrates excellent agreement between the two codes.

3.1.5 Passing data between models

Deterministic output data was transferred to Pandora with Excel files whereas probabilistic data was transferred with text files. The time steps in AMBER were selected automatically by a Laplace solver.

3.1.6 Rationales for using the code in SFR 1 SAR-08

The near and far field radionuclide transport calculations were in the SFR 1 SAR-08 project conducted by Enviros. As owners of the code Enviros have extensive knowledge of the use and application of the AMBER which is a suitable code for the task at hand. Amber is well known and widely used in assessments of this nature. The historical interaction with SKB and the safety analysis for SFR 1 means there is a good understanding of the issues associated with the application of AMBER to the specific details.

3.2 DarcyTools

3.2.1 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 used in DarcyTools V3.0. The grid system is an unstructured Cartesian grid which accurately represents objects and is read into the code as CAD-files.

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 /Svensson 2004/. Version 3.0 is the version used in SFR 1 SAR-08 and presently there is no updated documentation for this version. 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.

3.2.2 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 ground water 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.

The validity of the equations for solving the problem at hand is discussed in the SR-Can Process report for the Geosphere /SKB 2006c/

3.2.3 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.

3.2.4 Development process and verification

One of the tree documents mentioned above /Svensson 2004/ deals with verification and validation. About thirty basic 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.

3.2.5 Passing data between models

Flow factors for different climatic scenarios are presented in the model results report /Vidstrand et al. 2007/ and from there incorporated in the radionuclide transport models.

3.2.6 Rationales for using the code in SFR 1 SAR-08

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

3.3 Eikos

3.3.1 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 (see Section 3.6). In SAR-08, Eikos was used to perform sensitivity analysis of ecosystem and landscape models developed in Pandora. These models were used for derivation of activity inventories, concentrations and doses for SAR-08. Eikos was developed by Facilia AB and financed by Posiva OY and the Norwegian Radiation Protection Authority. The version used in SFR 1 SAR-08 is Eikos v2. The Eikos code is implemented as a toolbox in the commercial code Matlab and therefore it can be regarded as a category 4a code.

3.3.2 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.

3.3.3 Usage of the code

The Eikos code has a user guide /Ekström and Broed 2006/, which provides 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.

3.3.4 Development process and verification

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

3.3.5 Passing data between models

Eikos is integrated with the code Pandora and in that way no data is passed between the models externally.

3.3.6 Rationales for using the code in SAR-08

The models used for biosphere models in SAR-08 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 SAR-08.

3.4 Geoan

3.4.1 Introduction

The Geoan computer code is a numerical model for calculation of groundwater head, flow, velocity and transport in three dimensions, as well as surface water flow and surface water velocity. The mathematical model of the Geoan computer code is based on the continuum approach and the finite difference method.

A Geoan model fully integrates groundwater flow and surface water flow. The position of the groundwater surface and the actual recharge to the groundwater system is calculated by the model based on the surface topography, permeability of flow media, recharge, surface and groundwater flows, as well the transient state of the system studied.

By use of the pathway analyses module of the Geoan program, the program can calculate flow paths that are continuous in both the groundwater system and in the surface water system, and the flow paths may jump between both systems as given by the state of the system studied.

The computational grid of the Geoan computer code is a stiff grid that is partly unstructured. Boundary conditions of the cells of the grid may be determined by the computer code and change during procedure of solution (from saturated to unsaturated conditions etc). The groundwater surface may take place in any cell of the grid.

The Geoan code is used by Golder Associates for calculations of groundwater flow and transport, as the consultants of Golder Associated advices clients in the fields of nuclear waste, mining, contaminated land etc.

The Geoan computer code has been used by SKB in the SAFE project, considering the SFR 1-repository, as well as in several other projects carried out by SKB. The code includes special modules for the inclusion of a complex tunnel-system in the computational grid. Special modules are also available for detailed simulations of flow in closed tunnels, as well as modules for inverse modelling of inflow to drained tunnels. In addition special modules are available for modelling of the shore level progress, sediment accumulation as well as fully transient flow paths etc.

The code has also been used by Andra (the French nuclear waste management organisation) for research projects as well as for the safety assessment of a nuclear repository in fractured crystalline rock (the, Dossier 2005 – Granite, report by Andra). The code is at present applied by Golder Associates when advising Andra and SKB (as well as other clients).

The code was originally developed as a part of research work carried out by Dr Johan Holmén at the Uppsala University. The first version of the code was presented as a scientific thesis published by the Uppsala University 1992. At present the code is developed by Dr Holmén at Golder Associates.

The present version of the code carries number 07. The code is written in Fortran computer language and is compiled with the Intel Fortran compiler. Geoan is normally applied under the Windows operating system, Windows XP or Windows Server 2003. According to the SKB system of classifications, Geoan is a category 4b code.

3.4.2 Suitability of the code

The Geoan code was from the beginning developed for the specific purpose of simulation of groundwater flow. The mathematical descriptions applied by the code are therefore based on the appropriate physical laws and the code is adapted to the parameter ranges that occur when analysing groundwater and surface water flows.

- Groundwater flow is calculated by use of a differential equation based on Darcys law, see for example /Bear and Verruit 1987/. The equation is formulated by use of both implicit and explicit approaches. The equation is solved by use of the finite-difference method, and by application of iterative solvers. Flow paths in the groundwater system are calculated by use of a semi-analytic method; see /Pollock 1989/.
- Surface water flows and flow paths are calculated based on the topography as well as the recharge (precipitation minus evapotranspiraton) and the groundwater discharge. Velocity of the surface water flow is calculated by use of Manning's formula; see for example /Cedervall and Larsen 1976/. The Manning formula is solved by use of an iterative method.

A description of the code is given in /Holmén 1992/ and /Holmen 1997/. A users guide is also available, see /Holmén 2007/. Verification examples are given in /Holmén 1992/ and /Holmén 2007/.

The validity of the equations for solving the problem at hand is discussed in the SR-Can Process report for the Geosphere /SKB 2006c/.

3.4.3 Usage of the code

A description of how the code should be used is available in the users guide, /Holmén 2007/, in English.

The users guide contains the following:

- General information of the code and the system of menus.
- Detailed description of how to run a simulation.
- Detailed description of different boundary conditions and other special properties of the code.
- Detailed description of the format of the input files.
- Example of input files.
- Etc.

The Geoan computer code is normally used in the following way:

- An input file is created by the user; the input file describes the properties of the system studied. In addition to the main input file, Geoan may read and process information from other sources and computer programs, e.g. Fracman, Goldsim, Modflow, DarcyTools, Surfer, etc. Based on the data given to the Geoan program, Geoan will produce a number of output files that presents the system studied as defined by the user in the input files. Thereby allowing the user to check that the description of the system studied is correct.
- A simulation is carried out by use of Geoan.
- A large range of output files are created by Geoan, as specified by the user, these files include the results of the simulation.

The Geoan code does not include any visual tool for post-processing of the calculated results. Geoan produces output-files containing results that may be read, analysed, visualised and presented by use of several different computer programs e.g. Goldsim, Fracman, Tecplot, Surfer and Excel, etc.

3.4.4 Development process and verification

The development of the Geoan computer code follows established routines. The code is divided into a large number of separate modules that are linked together during compilation. The development is carried out in Microsoft Development Environment 2003, version 7.1.3. The code is written in the Fortran computer language and compiled by use of Intel Fortran version 9.1. At present the code is developed by Dr Holmén at Golder Associates.

The Geoan computer code (finite differences and stiff and partly unstructered grid) is verified against a large number of analytical solutions, and in addition considering test-cases for which there is no analytical solution available, the code is cross-verified against a computer code based on different methods (finite elements and adapted mesh). The Geoan code has also rather recently been cross-verified against two other computer codes used by SKB, the Connect Flow code and the Darcy Tools code. All new versions of the Geoan code are tested by use of analytical solutions and numerical cases. At present there is only one version of the code in use. Verification examples are given in /Holmén 1992/ and /Holmén 2007/.

3.4.5 Passing data between models

Deterministic results from the hydrogeology modelling were compiled in two reports /Holmén and Stigsson 2001ab/. Probabilistic results were transferred through text files.

3.4.6 Rationales for using the code in SFR 1 SAR-08

The Geoan computer code fully integrates groundwater flow and surface water flow. The code includes special modules for the inclusion of a complex tunnel-system in the computational grid. Special modules are also available for detailed simulations of flow in closed tunnels, as well as modules for inverse modelling of inflow to drained tunnels. In addition special modules are available for modelling of the shore level progress, sediment accumulation as well as fully transient flow paths etc.

3.5 Glacial isostatic adjustment software

3.5.1 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. Results from this modelling task performed within the SR-Can project were also used in SFR 1 SAR-08.

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, 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, 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/.

3.5.2 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 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.

3.5.3 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 /SKB 2006d/.

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.

3.5.4 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.

3.5.5 Passing data between models

Output data were transferred between the ice sheet-, GIA-, and permafrost simulations by text- or Excel files. Figure 3-1 shows the input and output data shared between the three models.

3.5.6 Rationales for using the code in SFR 1 SAR-08

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. This rationale is also valid for using the code in the safety assessment for SFR.

3.6 Pandora

3.6.1 Introduction

The landscape models, used in the biosphere assessments for SAR-08 were implemented in the software package Pandora /Åstrand et al. 2005/. Pandora is an extension of the well-known software 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 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. The version used in SFR 1 SAR-08 is Pandora rev 995. Since this code is an extension of commercial codes, it can be regarded as a category 4a code.

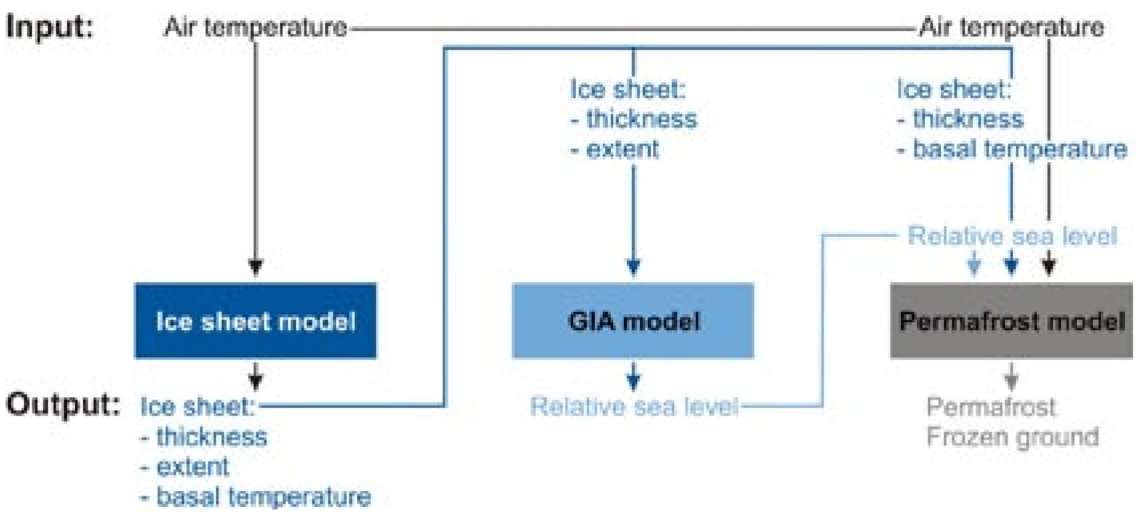

Figure 3-1. Input and output data shared between the three models used for modelling climate and climate related processes.

3.6.2 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 simulations for scenarios stretching over a long time span
- performing probabilistic simulations using the code Eikos (see Section 3.3).

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

3.6.3 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 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 a large list of solvers available in Simulink, including solvers that are appropriate for stiff systems of equations with discrete events. In SAR-08 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 function created in Matlab. Pandora is integrated with the code Eikos (see Section 3.3), which allows performing sensitivity and uncertainty analyses of the implemented models.

3.6.4 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/. These comparisons have shown that Pandora provides reliable solutions.

3.6.5 Passing data between models

Deterministic data from AMBER was transferred to Pandora with Excel files whereas probabilistic data was transferred with text files. Pandora is integrated with the code Eikos and in that way no data is passed between those two models externally.

3.6.6 Rationales for using the code in SAR-08

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.

3.7 Permafrost modelling code

3.7.1 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/deglaciation 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 2006d/. Results from this modelling task performed within the SR-Can project were also used in SFR 1 SAR-08. The version used for the modelling in SR-Can was version 1. 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 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, 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.

3.7.2 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/.

3.7.3 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.

There is no formally documented user's guide available.

3.7.4 Passing data between models

Output data were transferred between the ice sheet-, GIA-, and permafrost simulations by text- or Excel files. Figure 1 shows the input and output data shared between the three models.

3.7.5 Rationales for using the code in SFR 1 SAR-08

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. This rationale is also valid for using the code in the safety assessment for SFR.

3.8 PHREEQC

3.8.1 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 (≈ 25°C) aqueous geochemical calculations.

In the SR-Can project 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/). The work performed in the safety analysis of SFR 1 SAR-08 has been carried out using the version 2.13, which introduced multicomponent diffusion (MCD) and tools for modifying the porosity in a particular cell.

Since the code is an open source code, of a large user base and not written exclusively for the SAFE project, the code is regarded as a category 3 code. However, in order to study the influence of a varying temperature as well as non-fixed boundary conditions, additional routines were written, which means that models requiring this particular functionality can be considered as accomplished by a code classified as category 4a.

3.8.2 Suitability of the code

As the understanding of chemical behaviour of the near-field under different scenarios is of the main interest in the safety analysis of SFR 1 SAR-08, 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 and robust geochemical code. PHREEQC is based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, ion exchangers and sorption surfaces, but also includes the capability to model kinetic reactions with rate equations that are completely specified by the user 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/.

3.8.3 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 frequent answers and questions (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. The code has been slightly modified to handle variations in certain input parameters that normally are fixed. This modification is described in Section 3.8.4.

3.8.4 Development process and verification

The modification of the code consists of routines which automatically reset certain parameters that normally are fixed in a given input such as temperature, composition of boundary solution and porosity. Identical results can be achieved through manually resetting the parameters for each iteration, but this is obviously not feasible in a full scale simulation since each run could consist of at least 1000 iterations. The consistency with the non-modified code has been demonstrated by a comparison between results obtained by the non-modified code (through manual resetting of the affected parameters) and results obtained by the modified code (through automatic resetting of the same parameters) for a small number of iterations. The consistency has also been demonstrated through printing the value of the parameters for each iteration, using the programs own output routines. It is emphasized that all computational routines are left intact.

3.8.5 Passing data between models

No data is passed to or from this model, only assessments based on this or other models have been transfered.

3.8.6 Rationales for using the code in SFR 1 SAR-08

The SFR 1 SAR-08 team has selected the PHREEQC code for the safety assessment since it is useful to perform 1D dimensional transport calculations in combination with thermodynamical equilibrium calculations. The knowledge of this program is high and well supported.

3.9 UMISM

3.9.1 Introduction

The UMISM (University of Maine Ice Sheet Model) 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 is a dynamic ice-sheet model capable of simulating realistic ice sheets that are typically not in balance with climate (growing/shrinking). The simulations were performed using UMISM version as of May 2005.

UMISM is used in SR-Can for simulating 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. Results from this modelling task performed within the SR-Can project were also used in SFR 1 SAR-08.

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, 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).

3.9.2 Suitability of the code

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.

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/.

3.9.3 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 /SKB 2006d/. There is no formally documented user's guide available.

3.9.4 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.

3.9.5 Passing data between models

Output data were transferred between the ice sheet-, GIA-, and permafrost simulations by text- or Excel files. Figure 1 shows the input and output data shared between the three models.

3.9.6 Rationales for using the code in SFR 1 SAR-08

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.

These rationales are also valid for using the code in the safety assessment for SFR.

4 References

ANDRA, 2003. BIOSCOMP Project: Intercomparison Exercise between AQUABIOS, AMBER and MEPAS for the Calculation of the Transfers of Non-Radioactive Pollutants within the Biosphere. ANDRA Report Z RP 0ANT 03-029, December 2003.

Bassett S E, Milne G A, Mitrovica J X, Clark P U, 2005. Ice sheet and solid earth influences on far-field sea-level histories. Science, 309 (5736): 925–928.

Bear J, Verruit A, 1987. Modeling groundwater flow and pollution. D. Reidel publishing company, P.O.Box 17, 3300 AA Dorfrecht, Holland. ISBN 1-55608-014-X.

BIOMOVS II, 1996a. Validation Test for Carbon-14 Migration and Accumulation in a Canadian Shield Lake. BIOMOVS II Technical Report No. 14, published on behalf of the BIOMOVS II Steering Committee by the Swedish Radiation Protection Institute, Sweden.

BIOMOVS II, 1996b. Biosphere Modelling for Dose Assessments of Radioactive Waste Repositories: Final Report of the Complementary Studies Group. BIOMOVS II Technical Report No. 12, published on behalf of the BIOMOVS II Steering Committee by the Swedish Radiation Protection Institute, Sweden.

BIOMOVS II, 1996c. Model Validation Studies of Water Flow and Radionuclide Transport in Vegetated Soils Using Lysimeter Data. BIOMOVS II Technical Report No. 15, published on behalf of the BIOMOVS II Steering Committee by the Swedish Radiation Protection Institute, Sweden.

Cedervall K, Larsen P, 1976. Hydraulik för väg och vattenbyggare. ISBN 91-40-54300-5. Liber Läromedel 205 10 Malmö.

Chan T, Christiansson R, Boulton G S, Ericsson L O, Hartikainen J, Jensen M R, Mas Ivars D, Stanchell F W, Vistrand P, Wallroth T, 2005. DECOVALEX III BMT3/BENCHPAR WP4: The thermo-hydro-mechanical responses to a glacial cycle and their potential implications for deep geological disposal of nuclear fuel waste in a fractured crystalline rock mass. International Journal of Rock Mechanics and Mining Sciences, Vol. 42, pp 805–827.

Clark P U, Mitrovica J X, Milne G A, Tamisiea M E, 2002. Sea-level fingerprinting as a direct test for the source of global meltwater pulse IA. Science, 295 (5564): 2438–2441.

Côme B, Béon O, Albrecht A, Gallerand M O, Little R H, Strenge D L, 2004. Evaluating Multimedia Exposure Codes: the BIOSCOMP Exercise. In: Whelan G (ed.), Brownfields Multimedia Modelling and Assessment, WIT Press, Southampton, UK.

Enviros and Quintessa, 2005. AMBER White Paper: Fractured geosphere modelling.

Enviros and Quintessa, 2006a. AMBER 5 Reference Guide. Enviros, Culham and Quintessa, Henley-on-Thames, UK.

Enviros and Quintessa, 2006b. AMBER Users and References. Enviros Consulting Limited and Quintessa Limited.

Enviros and Quintessa, 2006c. AMBER 5 Release Note. Enviros Consulting Limited, Culham, and Quintessa, Henley-on-Thames, UK.

Enviros and Quintessa, 2006d. AMBER 5 Getting Started. Enviros, Culham and Quintessa, Henley-on-Thames, UK.

Ekström P-A, 2005. Eikos A Simulation Toolbox for Sensitivity Analysis. M.Sc. thesis, UPTEC Report IT 05 015, Uppsala University.

Ekström P-A, Broed R, 2006. Sensitivity Analysis Methods and a Biosphere. Test Case Implemented in Eikos. Posiva Working Report 2006-31.

Farrell W E, Clark J A, 1976. On postglacial sea level. Geophysical Journal of the Royal Astronomical Society, 46, 647–667.

Fastook J L, 1990. A map-plane finite-element program for ice sheet reconstruction: A steadystate calibration with Antarctica and a reconstruction of the Laurentide ice sheet for 18,000 BP. Computer Assisted Analysis and Modelling on the IBM 3090. H. U. Brown, IBM Scientific and Technical Computing Department, White Plains, New York.

Fastook J L, 1994. Modelling the Ice Age: The Finite-Element Method in Glaciology. Computational Science and Engineering 1(1): 55–67.

Fastook J L, Chapman J E, 1989. A map plane finite-element model: Three modelling experiments. Journal of glaciology 35(119): 48–52.

Fastook J L, Holmlund P, 1994. A glaciological model of the Younger Dryas event in Scandinavia. Journal of Glaciology 40(134), 125–131.

Fastook J L, Prentice M, 1994. A finite-element model of Antarctica: sensitivity test for meteorological mass-balance relationship. Journal of Glaciology 40(134): 167–175.

Ferry M, 2002. MIGAL. www.mfrdc.com.

Follin S, Stigsson M, Svensson U, 2005. Variable-density groundwater flow simulations and particle tracking – Numerical modelling using DarcyTools, Preliminary site description Simpevarp subarea – version 1.2. SKB R-05-11, Svensk Kärnbränslehantering AB.

Freund J, Lempinen A, 1994. A general purpose finite element solver. Report 40, Helsinki University of Technology, Institute of Computational Dynamics.

Gehrels W R, Milne G A, Kirby J R, Patterson R T, Belknap D F, 2004. Late Holocene sea-level changes and isostatic crustal movements in Atlantic Canada. Quaternary International, 120: 79–89.

Hartikainen J, 1994. Thermomechanical model for freezing soil and its computer implementation, Helsinki University of Technology, Department of Civil Engineering and Surveying, p 107, in Finnish. Master's thesis.

Hartikainen J, 2004. Permafrost modelling in DECOVALEX III for BMT3. In Eloranta E. ed., DECOVALEX III, 1999–2003. An international project for the modelling of coupled Thermo-Hydro-Mechanical processes for spent fuel disposal. Finnish national contributions. STUK-YTO-TR 209. Helsinki.

Hartikainen J, 2006. Numerical Simulation of Permafrost Depth at Olkiluoto. Posiva Oy. Working Report 2006-52.

Hartikainen J, Mikkola M, 1997. General thermomechanical model of freezing soil with numerical application. In Proceedings of the International Symposium on Ground Freezing and Frost Action in Soils, Luleå, Sweden, April 15–17, 1997, pp 101–105.

Hartikainen J, Mikkola M, 2006. Thermomechanical modelling for freezing of solute saturated soil. IUTAM Symposium on the mechanics of physicochemical and electromechanical interactions in porous media. J. M. Huyghe, Raats P.A.C. and Cowin, S. C. eds., 2006, pp 335–341.

Holmén J G, 1992. A three-dimensional finite difference model for calculation of flow in the saturated zone. Department of quaternary geology, Uppsala University, Uppsala, Sweden, ISBN 91-7376-119-2, ISSN 0348-2979.

Holmén J G, 1997. On the flow of groundwater in closed tunnels. generic hydrogeological modelling of a nuclear waste repository, SFL 3–5. Technical Report No. 97-10, Svensk Kärnbränslehantering AB.

Holmén J G, 2007. Geoan users guide. Version 42. Internal company document, available upon request from Golder Associates: E-mail: johan_holmen@golder.se.

Holmén JG, Stigsson M, 2001a. Modelling of future hydrogeological conditions at SFR. SKB R-01-02, Svensk Kärnbränslehantering AB.

Holmén JG, Stigsson M, 2001b. Details of predicted flow in deposition tunnels at SFR, Forsmark. SKB R-01-12, Svensk Kärnbränslehantering AB.

Holmlund P, Fastook J, 1995. A time dependent glaciological model of the Weichselian ice sheet. Quaternary International 27: 53–58.

Huybrechts P, Payne A J, 1996. The EISMINT benchmarks for testing ice-sheet models. Annals of Glaciology 23, 1–12.

IAEA, 2003a. Improvement of Safety Assessment Methodologies for Near Surface Disposal Facilities. Volume II: Test Cases. TECDOC to be published, International Atomic Energy Agency, Vienna.

IAEA 2003b. "Reference Biospheres" for Solid Radioactive Waste Disposal: Report of BIOMASS Theme 1 of the BIOsphere Modelling and ASSessment (BIOMASS) Programme. IAEA-BIOMASS-6, International Atomic Energy Agency, Vienna.

IAEA 2003c. The Use of Safety Assessment in the Derivation of Activity Limits for Disposal of Radioactive Waste to Near Surface Facilities. TECDOC to be published, International Atomic Energy Agency, Vienna.

Johnson J, 1994. A basal water model for ice sheets. Ph. D. Thesis, University of Minnesota.

Jones J, Vahlund F, Kautsky U, 2004. Tensit – a novel probabilistic simulation tool for safety assessments Tests and verifications using biosphere models. SKB TR-04-07, Svensk Kärnbränslehantering AB.

Kelly M, Cliffe K A, 2006. Validity document for COMP 23. SKB TR-06-76, Svensk Kärnbränslehantering AB.

Kendall R A, Mitrovica J X, Milne G A, 2005. On post-glacial sea level – II. Numerical formulation and comparative results on spherically symmetric models. Geophysical Journal International, 161 (3): 679–706.

Maul P R, Robinson P C, 2002. Exploration of Important Issues for the Safety of SFR 1 using Performance Assessment Calculations, SKI Report 02:62, June 2002.

Maul P R, Robinson P C, Avila R, Broed R, Pereira A, Xu S, 2003. AMBER and Ecolego Intercomparisons using Calculations from SR 97. SKI Report 2003:28/SSI Report 2003:11, Stockholm, August 2003.

Maul P R, Robinson P C, Broed R, Avila R, 2004. Further AMBER and Ecolego Intercomparisons. SKI Report 2004:05/SSI Report 2004:01, Stockholm, January 2004.

Mikkola M, Hartikainen J, 2002. Computational aspects of soil freezing problem. In Proceedings CD of the Fifth World Conress on Computational Mechanics, Vienna, Australia.

Milne G A, 1998. Refining models of the glacial isostatic adjustment process. Ph. D. Thesis, University of Toronto, Toronto.

Milne G A, Mitrovica J X, 1998. Postglacial sea-level change on a rotating Earth. Geophysical Journal International, 133 (1): 1–19.

Milne G A, Mitrovica J X, Davis J L, 1999. Near-field hydro-isostasy: the implementation of a revised sea-level equation. Geophysical Journal International, 139 (2): 464–482.

Milne G A, Davis J L, Mitrovica J X, Scherneck H G, Johansson J M, Vermeer M, Koivula H, 2001. Space-geodetic constraints on glacial isostatic adjustment in Fennoscandia. Science, 291 (5512): 2381–2385.

Milne G A, Mitrovica J X, Schrag D P, 2002. Estimating past continental ice volume from sea-level data. Quaternary Science Reviews, 21 (1–3): 361–376.

Milne G A, Mitrovica J X, Scherneck H G, Davis J L, Johansson J M, Koivula H, Vermeer M, 2004. Continuous GPS measurements of postglacial adjustment in Fennoscandia: 2. Modeling results. Journal of Geophysical Research, 109 (B2): B02412.

Milne G A, Long A J, Bassett S E, 2005. Modelling Holocene relative sea-level observations from the Caribbean and South America. Quaternary Science Reviews, 24 (10–11): 1183–1202.

Milne G A, Shennan I, Youngs B A R, Waugh A I, Teferle F N, Bingley R M, Bassett S E, Cuthbert-Brown C, Bradley S L, 2006. Modelling the glacial isostatic adjustment of the UK region. Philosophical Transactions of the Royal Society A – Mathematical Physical and Engineering Sciences, 364 (1841): 931–948.

Mitrovica J X, Peltier W R, 1991. On post-glacial geoid subsidence over the equatorial oceans. Journal of Geophysical Research, 96, 20053–20071.

Mitrovica J X, Tamisiea M E, Davis J L, Milne G A, 2001. Recent mass balance of polar ice sheets inferred from patterns of global sea-level change. Nature, 409 (6823): 1026–1029.

Mitrovica J X, Milne G A, 2002. On the origin of late Holocene sea-level highstands within equatorial ocean basins. Quaternary Science Reviews, 21 (20–22): 2179–2190.

Mitrovica J X, Milne G A, 2003. On post-glacial sea level: I. General Theory. Geophysical Journal International, 154 (2): 253–267.

Näslund J O, Rodhe L, Fastook J, Holmlund P, 2003. New ways of studying ice sheet flow directions and glacial erosion by computer modelling – examples from Fennoscandia. Quaternary Science Reviews 22:245–258.

Parkhurst D L, Appelo C A J, 1999. User's guide to PHREEQC (version 2) – a computer program for speciation, batch-reaction, one-dimensional transport and inverse geochemical calculations. USGS Water resources investigations report 99-4259, 312 p.

Payne A J, Huybrechts P, Abe-Ouchi A, Calov R, Fastook J L, Greve R, Marshall S J, Marsiat I, Ritz C, Tarasov L, Thomassen M P A, 2000. Results from the EISMINT model intercomparison: the effects of thermomechanical coupling. In Journal of Glaciology 46:153 227–238.

Pollock D W, 1989. Documentation of computer program to compute and display path lines using results from the U.S. Geological survey modular three-dimensional finite difference groundwater flow model, (Modpath manual). US Geological survey, 411 National Centre Reston, VA 22092, USA.

Robinson P C, 2008. AMBER White Paper: Modelling Rock Matrix Diffusion with AMBER Guidance Note. Quintessa, Henley on Thames.

Scott F A M, 1998. An Investigation into the Application of Compartmental Models in their Representation of Contaminants in the Environment. MSc Thesis, Centre for Environmental Technology, Imperial College of Science, Technology and Medicine, University of London.

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

SKB, 2006b. Buffer and backfill process report for the safety assessment SR-Can. SKB TR-06-18, Svensk Kärnbränslehantering AB.

SKB, 2006c. Geosphere process report for the safety assessment SR-Can. SKB TR-06-19, Svensk Kärnbränslehantering AB.

SKB, 2006d. Climate and climate related issues for the safety assessment SR-Can. SKB TR-06-23, Svensk Kärnbränslehantering AB.

Spalding D B, 1981. A General Purpose Computer Program for Multi-Dimensional One- and Two-Phase Flow. Mathematics and Computers in Simulation XXIII: pp 267–276.

Svensson U, 1991. Groundwater flow at Äspö and changes due to the excavation of the laboratory. SKB HRL Progress report 25-91-03, Svensk Kärnbränslehantering AB.

Svensson U, 2004. DarcyTools, Version 2.1. Verification and validation. SKB R-04-21, Svensk Kärnbränslehantering AB.

Svensson U, Kuylenstierna H-O, Ferry M, 2004a. DarcyTools, Version 2.1. Concepts, methods, equations and demo simulations. SKB R-04-19, Svensk Kärnbränslehantering AB.

Svensson U, Kuylenstierna H-O, Ferry M, 2004b. DarcyTools, Version 2.1. User´s guide. SKB R-04-20, Svensk Kärnbränslehantering AB.

Tamisiea M E, Mitrovica J X, Milne G A, Davis J L, 2001. Global geoid and sea level changes due to present-day ice mass fluctuations. Journal of Geophysical Research, 106 (B12): 30849–30863.

Tamisiea M E, Mitrovica J X, Davis J L, Milne G A, 2003. Long wavelength sea level and solid surface perturbations driven by polar ice mass variations: Fingerprinting Greenland and Antarctic ice sheet flux. Space Science Reviews, 108 (1–2): 81–93.

The MathWorks Inc. www.mathworks.com.

Thomson G, Herben M, Lloyd P, Rose D, Smith C, Barraclough I, 2007a. Implementation of Project SAFE in AMBER (SK0040004 v2)

Thomson G, Miller A, Smith G, 2007b. Radionuclide releases report for SAR08 (SK0040005).

Thomson G, Miller B, 2005. SFR 1 – Post closure radionuclide release and dose calculations. SKB R-05-81, Svensk Kärnbränslehantering AB.

Vidstrand P, Näslund J-O, Hartikainen J, Svensson U, 2007. Hydrogeological flux scenarios at Forsmark – Generic numerical flow simulations and compilation of climatic information for use in the safety analysis SFR 1 SAR-08. SKB R-07-63, Svensk Kärnbränslehantering AB.

Whitehouse P, Latychev K, Milne G A, Mitrovica J X, Kendall R, 2006. Impact of 3-D Earth structure on Fennoscandian glacial isostatic adjustment: Implications for space-geodetic estimates of present-day crustal deformations. Geophysical Research Letters, 33 (13): L13502.

Åstrand P-G, Jones J, Broed R, Avila R, 2005. Pandora technical description and user guide. Posiva Working Report 2005-64.