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Model summary report for the safety assessment SR-PSU

Svensk Kärnbränslehantering AB

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Preface

This report gives an overview of the computer codes used in a long-term radiation safety assessment of the low-and intermediate level waste repository SFR. It also describes the quality assurance procedures and the documentation related to each code. The report forms part of the SR-PSU safety assessment, which supports the application for a licence to extend the SFR repository in Forsmark.

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The report has been reviewed by Lena Zetterström Evins, SKB.

Stockholm, November 2014

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Summary

This report describes the computer codes used to carry out the modelling studies for the safety assessment SR-PSU, and the documentation and quality assurance (QA) processes associated with each code. A large number of numerical models have been used in SR-PSU to analyse the system and to show compliance. Therefore, an Assessment Model Flowchart (AMF) has also been constructed to summarise the different modelling tasks carried out and the codes applied, and to show how the models interact and how information is transferred between them.

The models applied in SR-PSU vary significantly in terms of their complexity, and some codes are commercial while others were developed, or adapted, for SKB assessments. Therefore, to account for the diversity of the codes, the following QA reporting requirements were identified:

- Demonstrate that the code is suitable for its purpose.
- Demonstrate that the code has been used properly.
- Demonstrate that the code development process has followed appropriate procedures and that the code produces accurate results.
- Describe how data are transferred between the different computational tasks.

Although the requirements are identical for all codes in the assessment, the measures used to demonstrate that the requirements have been fulfilled are different for different types of codes. Each assessment code is therefore presented along with a discussion on how these requirements are met.

Sammanfattning

Denna rapport beskriver de olika datorkoderna som använts inom den långsiktiga säkerhetsanalysen SR-PSU. Rapporten kvalitetsäkrar även koderna enligt metodik som ges i första kapitlet. Inom SR-PSU används ett antal olika koder i olika aktiviteter. För att förstå hur dessa olika aktiviteter hör ihop har en AMF (Assessment Model Flowchart) skapats. Från AMF:en har det gått att identifera hur aktiviteterna hör ihop och vilka aktiviteter som krävt speciella program.

Beräkningskoderna som används inom SR-PSU varierar mellan allt från kommersiella datorprogram med hundratusentals användare till program specifikt programmerade för säkerhetsanalyser med kanske bara ett tiotal aktiva användare och utvecklare. Detta ställer krav på kvalitetssäkringsmetodiken att vara både generell men samtidigt väldefinierad. Metodiken ställer följande krav på varje använd kod:

- Koden måste vara lämplig för det den används till inom SR-PSU.
- Koden måste ha använts på korrekt sätt inom SR-PSU.
- Det måste visas att koden har programmerats på korrekt sätt och att den ger korrekta resultat.

Även om samma krav ställs kan inte bevisen för att kraven uppfylls redovisas på samma sätt för alla koder. Det vanligaste skälet för detta är att flera av programmen inte har öppen källkod och att man då istället får förlita sig på till exempel kontrollberäkningar med andra program. De olika metoderna att bevisa kodens lämplighet redovisas i varje kods kapitel.

Contents

1 Introduction

1.1 Background

The final repository for short-lived radioactive waste (SFR) located in Forsmark, Sweden is used for the final disposal of low- and intermediate-level operational waste from Swedish nuclear facilities. SKB plans to extend SFR to host waste from the decommissioning of the nuclear power plants and other nuclear facilities. Additional disposal capacity is needed also for operational waste from nuclear power units in operation since their operation life-times have been extended compared with what was originally planned.

The SFR repository includes waste vaults underground together with buildings above ground that include a number of technical installations. The underground part of the existing facility (SFR 1) is situated at 60 metres depth in the rock and is located below the Baltic Sea. SFR 1 comprises five waste vaults with a disposal capacity of approximately 63,000 m^3. The extension (SFR 3)[1] will be built at 120 metres depth and will have a disposal capacity of 108,000 m^3 in five new waste vaults plus one new vault for nine boiling water reactor pressure vessels, see Figure 1-1.

The long-term post closure safety of the whole SFR has been assessed and documented in the SR-PSU Main report with supporting documents, see Section 1.2. The Main report is part of SKB's licence application to extend and continue to operate SFR. This report is a main reference and describes the computer codes used to carry out the modelling studies for the long-term safety assessment SR-PSU, and the documentation including the quality assurance processes related to each code.

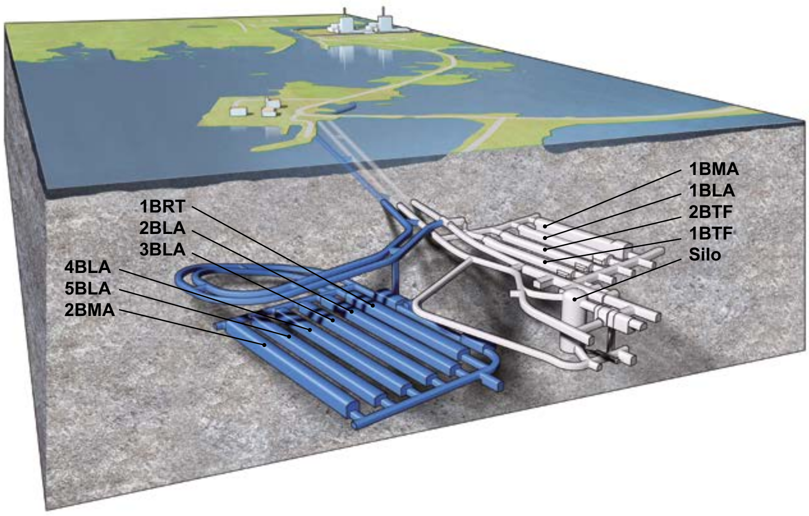

Figure 1-1. *Schematic illustration of SFR. The grey part is the existing repository (SFR 1) and the blue part is the planned extension (SFR 3). The waste vaults in the figure are the silo for intermediate-level waste, 1–2BMA vaults for intermediate-level waste, 1–2BTF vaults for concrete tanks, 1–5BLA vaults for low-level waste and the BRT vault for reactor pressure vessels.*

[1] The extension is called SFR 3 since the name SFR 2 was used in a previous plan to build vaults adjacent to SFR 1 for disposal of reactor core components and internal parts. The current plan is to dispose of this waste in a separate repository.

1.2 Report hierarchy in the SR-PSU safety assessment

The applied methodology for the long-term safety comprises ten steps and is described in Chapter 2 of the SR-PSU Main report. Several of the steps carried out in the safety assessment are described in more detail in supporting documents, so called main references that are of central importance for the conclusions and analyses in the **Main report**. The full titles of these reports together with the abbreviations by which they are identified in the following text (abbreviated names in bold font) together with short comments on the report contents are given in Table 1-1.

There are also a large number of additional references. The additional references include documents compiled within SR-PSU, but also documents compiled outside of the project, either by SKB or equivalent organisations as well as in the scientific literature. Additional publications and other documents are referenced in the usual manner.

A schematic illustration of the safety assessment documents is shown in Figure 1-2.

1.3 This report

The purpose of this report is to give an overview of the modelling tasks and computer codes used in the long term radiation safety assessment for SFR (SR-PSU) and the quality assurance procedures and documents relating to the codes. More specifically, the report contains:

- An Assessment model flow chart (AMF) that describes the modelling tasks in SR-PSU and how the different modelling tasks are connected.
- The principles behind the QA measures regarding the codes and the calculations.
- A brief presentation of each code identified in the AMF. The presentation is outlined in Section 2.5. The presentations also include a justification for each code.

The three process reports, **Waste process report**, **Barriers process report** and **Geosphere process report** together with the **Data report** give the rationale for including a certain process in the modelling and for selecting the input data, respectively.

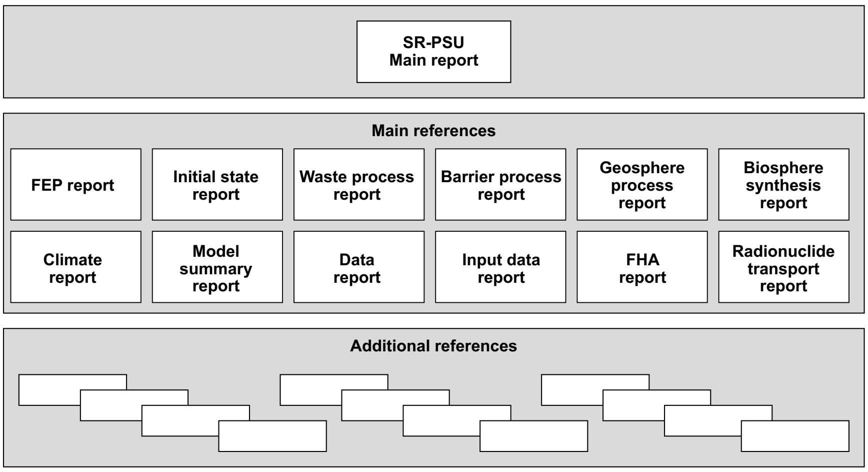

__Figure 1-2.__ The hierarchy of the Main report, main references and additional references in the SR-PSU long-term safety assessment. The additional references either support the Main report or any of the main references.

Table 1-1. Main report and main references in the SR-PSU long term safety assessment. All reports are available at www.skb.se

Abbreviation used when referenced in this report	Full reference	Comment on content
Main report	**Main report, 2014**. Safety analysis for SFR. Long-term safety. Main report for the safety assessment SR-PSU. SKB TR-14-01, Svensk Kärnbränslehantering AB.	This document is the main report of the SR-PSU long-term post-closure safety assessment for SFR. The report is part of SKB´s licence application to extend and continue to operate SFR.
Barriers process report	**Engineered barriers process report**, **2014**. Engineered barrier process report for the safety assessment SR-PSU. SKB TR-14-04, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the engineered barriers that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled a particular way in the safety assessment.
Biosphere synthesis report	**Biosphere synthesis report**, **2014**. Biosphere synthesis report for the safety assessment SR-PSU. SKB TR-14-06, Svensk Kärnbränslehantering AB.	Describes the handling of the biosphere in the safety assessment. The report summarises site description and landscape evolution, FEP handling, exposure pathway analysis, the radionuclide model for the biosphere, included parameters, biosphere calculation cases and simulation results.
Climate report	**Climate report**, **2014**. Climate and climate-related issues for the safety assessment SR-PSU. SKB TR-13-05, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of climate and climate-related processes that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. The report also describes the climate cases that are analysed in the safety assessment.
Data report	**Data report, 2014.** Data report for the safety assessment SR-PSU. SKB TR-14-10, Svensk Kärnbränslehantering AB.	Qualifies data and describes how data, including uncertainties, that are used in the safety assessment are quality assured.
FEP report	**FEP report, 2014.** FEP report for the safety assessment SR-PSU. SKB TR-14-07, Svensk Kärnbränslehantering AB.	Describes the establishment of a catalogue of features, events and processes (FEPs) that are of potential importance in assessing the long-term functioning of the repository.
FHA report	**FHA report**, **2014**. Handling of future human actions in the safety assessment SR-PSU. SKB TR-14-08, Svensk Kärnbränslehantering AB.	Describes radiological consequences of future human actions (FHA) that are analysed separately from the main scenario, which is based on the reference evolution and less probable evolutions.
Geosphere process report	**Geosphere process report**, **2014**. Geosphere process report for the safety assessment SR-PSU. SKB TR-14-05, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the geosphere that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled a particular way in the safety assessment.
Initial state report	**Initial state report**, **2014**. Initial state report for the safety assessment SR-PSU. SKB TR-14-02, Svensk Kärnbränslehantering AB.	Describes the conditions (state) prevailing in SFR after closure. The initial state is based on verified and documented properties of the repository and an assessment of the evolution during the period up to closure.
Input data report	**Input data report**, **2014**. Input data report for the safety assessment SR-PSU. SKB TR-14-12, Svensk Kärnbränslehantering AB.	Describes the activities performed within the SR-PSU safety assessment and the input data used to perform these activities.
Model summary report	**Model summary report**, **2014**. Model summary report for the safety assessment SR-PSU. SKB TR-14-11, Svensk Kärnbränslehantering AB.	Describes the calculation codes used in the assessment.
Radionuclide transport report	**Radionuclide transport report**, **2014**. Radionuclide transport and dose calculations for the safety assessment SR-PSU. SKB TR-14-09, Svensk Kärnbränslehantering AB.	Describes the radionuclide transport calculations carried out for the purpose of demonstrating fulfilment of the criterion regarding radiological risk.
Waste process report	**Waste process report, 2014.** Waste form and packaging process report for the safety assessment SR-PSU. SKB TR-14-03, Svensk Kärnbränslehantering AB.	Describes the current scientific understanding of the processes in the waste and its packaging that have been identified in the FEP processing as potentially relevant for the long-term safety of the repository. Reasons are given in the process report as to why each process is handled in a particular way in the safety assessment.

2 Quality assurance principles for the computer codes

This chapter describes the quality assurance principles relating to the software and computer codes used in the safety assessment SR-PSU. An assessment model flow chart (AMF) is presented to provide an overview of the modelling activities and the flow of information between them. Different categories of computer code are then defined and the QA requirements are given for each category. Finally, a template for describing the different codes is presented.

2.1 Assessment model flow chart

The AMF constructed for the SR-PSU safety assessment illustrates how the modelling tasks in the assessment are connected. 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. In addition to the models presented in the flow chart, minor calculations might have been performed, for instance when post-processing results or when preparing input data. These are not included in the present document, as explained in Section 2.3.

2.2 Computer codes and AMF activities

In Table 2-1 the computer codes used for the modelling activities shown in the AMF (Appendix A) are given. For each modelling activity the used computer code and the background reports presenting the results of the calculations performed within the SR-PSU safety assessment are given in Table 2-1. The computer codes are described in Sections 3.1 to 3.14.

Table 2-1. SR-PSU Modelling activities from AMF (see Appendix A), computer codes used and background reports for modelling results.

Modelling activity	Section Computer code	AMF Outputs	Background report(s)
Waste			
Corrosion of reactor pressure vessels	3.7 Ecolego	95	**Radionuclide transport report**
Near field			
Bitumen swelling assessment	3.5 Comsol Multiphysics	150	von Shenck and Bultmark 2014
Evolution of repository pH	3.14 PHREEQC	51, 133, 174, 206	Cronstrand 2014
Evolution of repository redox	3.14 PHREEQC	49	Duro et al. 2012
Near-field hydrology	3.5 Comsol Multiphysics	50, 104, 109, 153, 176	Abarca et al. 2014
Rebar corrosion and chemical degradation of concrete	3.13 PHAST	38	Höglund 2014
RN transport in water phase	3.7 Ecolego	76	**Radionuclide transport report**
Seismic load	3.2 ADINA	25	Georgiev 2013
Geosphere			
Hydrogeology	3.6 Darcy Tools	7, 9, 11, 12, 84, 135	Odén et al. 2014
RN transport in water phase	3.7 Ecolego	16	**Radionuclide transport report**
Rock fallout and EDZ	3.1 3DEC	6, 26	Mas Ivars et al. 2013
Climate			
Climate cases representing prolonged interglacial conditions	3.4 CCSM4, 3.8 LOVE-CLIM, 3.10 Numerical GIA model, 3.11 Numerical permafrost model	13, 18, 65, 72, 74, 128	Brandefelt et al. 2013, Goosse et al. 2010, **Climate report**, Hartikainen et al. 2010
Minimum air temperature in next 60,000 years	3.4 CCSM4, 3.8 LOVE-CLIM	66, 210	Brandefelt et al. 2013, Goosse et al. 2010
Potential for permafrost	3.4 CCSM4, 3.8 LOVE-CLIM, 3.11 Numerical permafrost model	188	Brandefelt et al. 2013, Goosse et al. 2010, Hartikainen et al. 2010
Shore-level evolution	3.10 Numerical GIA model	190	**Climate report**
Weichselian glacial cycle climate case representing natural variability	3.10 Numerical GIA model, 3.11 Numerical permafrost model	191, 196	**Climate report**, Hartikainen et al. 2010
Weichselian ice-sheet development	3.12 Numerical ice sheet model (UMISM)	69, 142, 193	**Climate report**
Weichselian permafrost development	3.4 CCSM4, 3.8 LOVE-CLIM	192	Brandefelt et al. 2013, Goosse et al. 2010
Weichselian shore-level evolution	3.10 Numerical GIA model	194	**Climate report**
Biosphere			
Biosphere object identification	3.3 ArcGIS	103	**Biosphere synthesis report**, Brydsten and Strömgren 2013
Landscape modelling	3.3 ArcGIS	1, 52, 54, 99, 164	**Biosphere synthesis report**, Strömgren and Brydsten 2013, Sohlenius et al. 2013
RN transport and dose	3.7 Ecolego	212	**Radionuclide transport report**
Surface hydrology	3.9 MIKE SHE	138, 173	**Biosphere synthesis report**, Werner et al. 2013a

2.3 Types of codes used in the assessment

As shown in the AMF, a large number of modelling activities support the SR-PSU safety assessment. The different codes used range in complexity from simple routines written in scripts languages in commercially available codes such as MATLAB or Microsoft Excel, to large programs (thousands of lines) written in programming languages such as C++ and Fortran. The origins of the codes also differ substantially; some are commercial, have a large world-wide user base and can be regarded as well tested, while others were written exclusively for SKB safety assessments. The source codes of codes developed for SKB safety assessments are generally available for review, while the quality assurance procedures of the developer have to be accepted for commercially available codes. A differentiated approach to quality assurance, with adaptations to the types of codes used in the assessment, is thus required.

The following categories of computer codes have been identified:

1. Commercial system software such as operating systems, compilers and database software. Although necessary for the assessment, these codes are not regarded as assessment codes and are hence not included in the AMF or in the model documentation.
2. Software used to solve problems that can be verified by simple calculations. This category also includes codes used for unit conversion and pre- and post-processing of data. This category is also not included in this document.
3. Wide-spread commercial or open source codes. These have a large user base and are therefore considered to be sufficiently well tested. Therefore, the need for verification tests is limited within SR-PSU. These codes are not written exclusively for the safety assessment and the user of the code may in many cases be an expert on using the code. The documentation for these codes is generally extensive but may not be 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 independently of the SR-PSU project. Using these codes for assessment calculations implies that the QA procedures used by the developer of the codes are accepted.

4a. Modified commercial codes. Some commercially available codes allow the user to add functionality to the original code through standardised methods with the extension working as an integrated part of the original code. Since functionality is added, there is a greater need for verification studies for these codes than for codes in the previous category. Verification studies within SR-PSU are however only required for the added functionality and not for the original code. Using these codes for assessment calculations implies that the QA procedures used by the developer of the codes are accepted.

4b. Calculations performed with codes developed within the safety assessment, frequently written in languages such as C++ and Fortran. In general, these codes are written with the safety assessment application in mind and have a considerably smaller user base than codes in category 3. There is therefore a greater need for verification of these codes.

There may be cases where it is not evident whether a code should be in category 4a or 4b. Codes developed within the project may for instance contain 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 code that is not part of the original code) is the same for 4a and 4b. Based on these categories, the quality assurance procedures for each type of code are presented in Section 2.4.

2.4 Requirements for assessment codes

There are four basic requirements for the quality assurance of each code and its application:

- The code is shown to be suitable for its purpose – required for all categories.
- The code has been used properly – required for all categories.
- The code development process has followed appropriate procedures and that the code produces accurate results – this applies to category 4 codes since these have been developed by the implementer. For codes in categories 1 to 3, the procedures of the developer are accepted.
- A description of how data are transferred between the different computational tasks is given. Note that this does not include a description on how data are handled internally by the model (covered in point 1 and 2 above and in documents where the calculations are presented). Due to the large number of modelling activities, it is possible that data are transferred between activities in many different ways.

The requirements are described further in Section 2.5, within the template for reporting the codes in this model summary report. Four of the six headings in the template relate directly to the basic requirements stated above.

2.5 Template used for reporting the codes in Chapter 3

2.5.1 Introduction

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

- A brief description of the problem solved by the code in the SR-PSU assessment.
- The usage of the code in previous performance assessments (at SKB or elsewhere) and, if relevant, which previously used code it supersedes and the reason for this.
- The version of the code and the platform used in the assessment calculations.
- The category chosen for the code based on the definition in Section 2.3, and a description of how the code has been developed.

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

2.5.2 Suitability of the code

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

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

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

2.5.3 Usage of the code

It is necessary to show that sufficient information on the usage of the code is available. This section should contain the following:

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

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

2.5.4 Development process and verification

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

2.5.5 Handling of input data, computational results and scripts

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

2.5.6 Rationale for using the code in the assessment

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

3 Description of the codes

This chapter provides a description of the codes used in the SR-PSU safety assessment, as shown in the AMF (Appendix A and Table 2-1), following the template given in Section 2.5.

3.1 3DEC

3.1.1 Introduction

3DEC is a three-dimensional numerical program that simulates the mechanical response of discontinuous media subjected to either static or dynamic loading. It uses the distinct element method for discontinuum modelling (Itasca 2003, 2007), and is based on the extensively-tested two-dimensional version, UDEC (Itasca 2005).

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 waste. Both static and dynamic analyses for deep underground openings have been performed, see for instance Stephansson et al. (1991), Sjöberg (1992) and Senseny (1993). 3DEC has been used by SKB in earlier studies regarding thermo-mechanical effects on the bedrock around a deep repository (Hakami et al. 1998). Many of the rock mechanics analyses referred to in SR 97 were conducted using 3DEC. In SR-Site and SR-Can, 3DEC was used for static analyses of mechanical effects on rock and rock fractures within and around the repository (Fälth and Hökmark 2007, Hökmark et al. 2010), and for dynamic analyses of fracture shear displacements induced by postglacial fault movements (Fälth and Hökmark 2006, Fälth et al. 2010). 3DEC is currently used by engineers, consultants and researchers in more than 30 countries around the world.

For SR-PSU safety assessment, 3DEC was used to carry out 3D numerical analyses of the stability of the SFR rock vaults after excavation and over the following 10,000 years (Mas Ivars et al. 2013). The model examined rock fallout and the stability of the rock pillar between repository vaults.

The SR-PSU 3DEC analyses were run on Windows-based PC-systems using 3DEC version 4.20. 3DEC is a commercial code with a large user base, and so is a category 3 code.

3.1.2 Suitability of the code

3DEC is designed for mechanical analyses 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 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.

3.1.3 Usage of the code

The documentation of 3DEC (Itasca 2003, 2007) is provided by Itasca Consulting Group Inc. The documentation contains a complete description of the code and the constitutive models that are implemented.

3.1.4 Development process and verification

The formulation and development of the distinct element method, which is the core of 3DEC, begun in 1971 (Cundall 1971) and has been on-going 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. The documentation can be accessed at the Itasca Website: http://www.itascacg.com/software/3dec.

3.1.5 Handling of input data, computational results and scripts

All input data (geometries, material data, initial- and boundary conditions, solution strategies) are entered as text files. The input files specify the results that will be monitored and recorded during the analysis. These results can be plotted or exported as text files. 3DEC has a plotting tool, which can be used to build the model (geometry, application of boundary conditions etc). The plotting tool also has a wide range of possibilities for producing vector- and contour plots for the post-processing of the results.

The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.1.6 Rationales for using the code in the assessment

The 3DEC code was tested thoroughly for the SR-Site project (see Fälth and Hökmark 2007 and Hökmark et al. 2010) and was shown to be suitable for its intended purpose. The successive development of later models and scripts provides traceability. 3DEC is considered to be the best option for modelling rock stability over time.

3.2 ADINA

3.2.1 Introduction

The ADINA software (ADINA 2010) is a finite element program designed for stress analysis of solids (2D and 3D) and structures in statics and dynamics. The analysis can be linear or highly nonlinear, including effects of material nonlinearities, large deformations and contact conditions. ADINA has not been used in safety assessments previously.

ADINA version 8.9.1 running on Windows 7 was used in SR-PSU to estimate the SFR Silo's ability to withstand earthquake loads. There was no predefined load that the structure was required to withstand, so the aim was to find the critical load instead – the load level for which the integrity of the structure is compromised. The estimation of the capacity is nevertheless restricted by the assumptions and simplifications that were made in the modelling and analysis phases (see Georgiev 2013).

Since ADINA is a wide-spread commercial software with a large user base it is classified as a category 3 code.

3.2.2 Suitability of the code

ADINA is a wide spread commercial code used for all sorts of stress analyses of solids and structures. The program implements finite element models to solve these stress analysis problems and is used within many different industries.

The usage in SR-PSU, further described in Georgiev (2013), is to analyse the SFR Silo's ability to withstand stresses caused from earthquake pulses of different magnitudes. The software does so by solving a large system of partial differential equations arranged in a finite element model mesh grid reflecting the silo geometries. All the equations are given in Georgiev (2013) Appendix A.

3.2.3 Usage of the code

In the ADINA manual (ADINA 2010) the program is described in detail, with several examples. The webpage of the program, http://www.adina.com , also contains further examples as well as a FAQ.

3.2.4 Development process and verification

ADINA is a commercial software developed by American company ADINA R&D. The code is widely used and its algorithm has been checked in several scientific publications (see ADINA website http://www.adina.com/) and through the example files distributed with the computer program. No modifications of the code has been reported in SR-PSU.

3.2.5 Handling of input data, computational results and scripts

All input and output files to ADINA are ASCII text files, which can be read and modified with standard spreadsheet tools such as Microsoft Excel. For the given problem to be analysed the ADINA program needed the geometries of the Silo structure as well as the mechanical properties of the Silo materials (e.g. concrete with and without reinforcement, pure bentonite and bentonite mixed with sand).

The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.2.6 Rationales for using the code in the assessment

The ADINA code was selected for the SR-PSU safety assessment since it is able to model stress analysis using the finite element method, which was a requirement to be able to assess an earthquake scenario. The program is widely used, well suited to nuclear waste disposal scenarios and well supported.

3.3 ArcGIS

3.3.1 Introduction

The ArcGIS code is a commercial geographic information system (GIS) code that is developed by ESRI. The two versions ArcGIS 9.3 and ArcGIS 10.2 have been used within the SR-PSU modelling. The system is certified for Windows XP Professional Service Pack 3 (32 bit), Windows Vista Business Service Pack 2 (64 bit) and Windows 7 Professional Service Pack 1 (32 and 64 bit). In the SR-PSU modelling both the Windows XP and Windows 7 platforms have been used.

ArcGIS has been used as a supportive tool in several fields and specifically it constituted the main modelling tool when developing the digital elevation model (DEM), the vegetation model and the regolith models (**Biosphere synthesis report**, Strömgren and Brydsten 2013, Sohlenius et al. 2013). Arc GIS was also used in the landscape modelling, describing the past, present and future landscape in Forsmark in terms of land use and shoreline displacement (**Biosphere synthesis report**, Brydsten and Strömgren 2013).

3.3.2 Suitability of the code

ArcGIS is an advanced geographical information system. Using the extension tool packs Spatial analyst and 3D analyst it is a powerful tool for analysis of spatial data. The Spatial analyst tool pack enables thorough analysis of spatial distributed data in a range from basic algebra operations to advanced geostatistical operations. The possibility to build up flow chart models facilitates the documentation, and enables the end user to track each individual operation made to the original data.

3.3.3 Usage of the code

The ArcGIS user manual and reference guide gives a detailed description of the individual tools and dialogs the user encounters when working with the ArcGIS user interface. The documents also includes detailed descriptions of examples used in the ArcGIS modelling system (http://help.arcgis.com/en/arcgisdesktop/10.0/help/).

Input data are supplied to the code as text files, shape-files or ESRI-grid files. Result files are ESRI-grid files or shape-files. ESRI-grid files and shape-files can also directly be converted to numerous formats.

3.3.4 Development process and verification

ESRI's ArcGIS is a geographic information system (GIS) used for: creating and using maps; compiling geographic data; analysing spatial distributed information; sharing and discovering geographic information; using maps and geographic information in a range of applications; and managing geographic information in a database. In 1999 the new platform ArcGIS 8.0 was released. ArcGIS replaced the previous software version from ESRI; ArcView. The current version is ArcGIS 10.2.1

ArcGIS has a close integration with SKB's GIS-database. This ensures an acceptable level of quality as well as a high level of traceability for the input data to the model and the result.

3.3.5 Handling of input data, computational results and scripts

Several ArcGIS models (DEM, vegetation and regolith model) from the SR-Site Assessment (SKB 2010c) have been further developed and elaborated in SR-PSU in order to include new data and findings. The resulting GIS models and maps are stored in the SKB GIS database.

3.3.6 Rationales for using the code in the assessment

ArcGIS is used in SR-PSU for terrain models, vegetation models, regolith models and landscape development models. Many of the models are used as input to other modelling activities within SR-PSU, e.g. surface hydrological modelling with MIKE SHE and geohydrological modelling with Darcy tools. ArcGIS is a well established tool that is suitable for analysis of geographical data. The flexibility in data formats and the possibility to import and export data on several data formats make the code easily compatible with other modelling tools used in the assessment.

3.4 CCSM4

3.4.1 Introduction

The National Center for Atmospheric Research (NCAR) Community Climate System Model version 4 (CCSM4) is a fully coupled ocean–atmosphere–land–sea–ice model that may be employed for the simulation of past, present and future climates (Gent et al. 2011). It includes the dynamics of the atmosphere (CAM4), ocean and sea-ice (POP2 and CICE4) and land (CLM4).

CCSM4 was used, in combination with other published intercomparison studies, for estimating the uncertainty in the minimum near-surface air temperature in Forsmark in the next 60,000 years simulated with the LOVECLIM Earth system model of intermediate complexity (see Section 3.8), see the **Climate report**, Section 2.1.4. The sensitivity of the simulated climate in Forsmark to the model formulation is estimated by comparing the CCSM4 and LOVECLIM simulations, and using the results of published climate model intercomparison studies.

The CCSM4 code was developed by the international climate research community over several decades. This version is an improved version of the previous version CCSM3, which was used in SR-Site.

The CCSM4 code is a category 3 code, written in Fortran, C and C++. The simulations were performed on the Ekman supercomputer at the Parallell Computing Centre (PDC) at the Royal institute of technology (KTH) in Stockholm.

3.4.2 Suitability of the code

The atmosphere component is the Community Atmosphere Model version 4, CAM4, an atmospheric general circulation model with a finite volume core and a horizontal grid with a resolution of ~2°. The atmosphere has 26 vertical levels from the surface to approximately 2 hPa.

The land component is the Community Land Model version 4 (CLM4), which uses the same horizontal resolution as the atmosphere component.

The ocean component is based on the Parallel Ocean Program version 2 (Smith et al. 2010), which has a horizontal resolution of ~1°. There are 60 depth layers (vs. 25 depth layers in the previous version CCSM3).

The sea ice module is the Community Ice Code version 4, which employs the same horizontal grid as the ocean module.

Compared to the previous version, CCSM3, CCSM4 includes several significant developments and improvements, including carbon–nitrogen cycling, a much improved representation of atmospheric deep convection, a new freeze-dry scheme for polar low clouds, an improved representation for surface runoff and frozen soil, an improved parameterisation for near-surface oceanic eddies, new parameterisations for sub-meso scale mixed layer eddies and ocean overflows, and a new radiative transfer scheme for sea ice/snow (Gent et al. 2011). These changes improve the model representations of e.g. the frequency of ENSO variability, of polar cloud cover, of the penetration of the North Atlantic meridional overturning circulation, of land water storage, and of the Arctic sea ice concentration and its trend (Gent et al. 2011). An ensemble of twentieth-century simulations produces a good match to the observed September Arctic sea ice extent from 1979 to 2005 (Gent et al. 2011). The CCSM4 ensemble mean increase in globally averaged surface temperature between 1850 and 2005 is larger than the observed increase by about 0.48°C. This is consistent with the fact that CCSM4 does not include a representation of the indirect effects of aerosols, although other factors may come into play.

3.4.3 Usage of the code

In the SR-PSU assessment, the CCSM4 code was used by scientists with experience in climate modelling, and the simulated climate was compared with data provided by the model developers. The version used in SR-PSU is described in Gent et al. (2011).

The CCSM4 model requires a large number of input data and parameters. In the simulations performed for SR-PSU, all input data and parameters were set at their default values (representing year 1850 AD) as given by the developers of the code, except for two sets of parameters. These were: orbital year (which determines the latitudinal and seasonal distribution of incoming solar radiation) and atmospheric greenhouse gas concentrations (carbon dioxide, methane and nitrous oxide), which were changed in order to simulate future conditions. Two simulations were performed with the model run with constant forcing and boundary conditions. The time step used in the different model components varies, but is less than one day for all components. Details of model setups and input data for individual SR-PSU simulations are found in Brandefelt et al. (2013).

Output data on a number of atmospheric and oceanic variables, such as air temperature and ocean water temperature and salinity, are saved at monthly and annual resolution in NetCDF format. These are given in a latitude–longitude grid. The atmospheric and vegetation variables are given in a regular ~2° latitude–longitude grid, whereas the oceanic variables are given in a regular ~1° latitude-longitude grid.

3.4.4 Development process and verification

The CCSM4 code was developed by the international climate research community over several decades. The version of the code used for SR-PSU is described in Gent et al. (2011).

CCSM4 has been used in an extensive range of research projects. It was included in the Climate Modelling Intercomparison Project 5 (CMIP5; http://cmip-pcmdi.llnl.gov/cmip5/) in support of the fifth assessment report of the Intergovernmental Panel on Climate Change (IPCC 2013; www.ipcc.ch). It was also included in the Paleoclimate Modelling Intercomparison Project 3 (PMIP3; www.pmip3.lsce.fr).

CCSM4 produces a reasonably realistic modern climate (Gent et al. 2011). However, it still has significant biases, such as the mean precipitation distribution in the tropical Pacific Ocean, too much low cloud in the Arctic, and the latitudinal distributions of shortwave and longwave cloud forcings (Gent et al. 2011). Further a warm bias is found in annual average near surface temperature over land, with a maximum of more than 5°C in eastern Europe and central Eurasia (Gent et al. 2011).

Equilibrium climate sensitivity (ECS) is defined as the global equilibrium surface-air-temperature change in response to instantaneous doubling of atmospheric CO_2 concentration. The ECS is 3.1°C for CCSM4 when run at the same resolution as in the present study, which is close to the average of the ECS of 2.0–4.5°C for the Atmosphere-Ocean General Circulation Models (AOGCMs) in IPCC AR4 and the ECS of 2.1–4.7°C for the AOGCMs in CMIP5, see Brandefelt et al. (2013).

3.4.5 Handling of input data, computational results and scripts

Data from CCSM4 was compared with data from LOVECLIM in order to estimate the uncertainty in the near-surface air temperature in Forsmark simulated by LOVECLIM. No data from CCSM4 were explicitly delivered to other SR-PSU activities.

3.4.6 Rationales for using the code in the assessment

The CCSM4 code was used, in combination with other published intercomparison studies, for estimating the uncertainty in the minimum near-surface air temperature in Forsmark in the next 60,000 years simulated with LOVECLIM Earth system model of intermediate complexity (see Section 3.4.2). The code was selected for the SR-PSU safety assessment since it is one of the world-leaders in its field.

3.5 Comsol Multiphysics

3.5.1 Introduction

Comsol Multiphysics is a commercial finite element software for solving coupled partial differential equations. In the SR-PSU the code has primarily been used to model the near-field hydrology (Abarca et al. 2013, 2014). Comsol has also been used for structural mechanics calculations to assess how swelling waste may affect concrete barriers (von Schenck and Bultmark 2014). Comsol Multiphysics has not been used in previous safety assessments.

Comsol Multiphysics v4.3a (Comsol 2012a) running under Windows has been used in the assessment calculations. The following add-on products have been used in addition to the base package:

- CAD Import Module (Comsol 2012b).
- Subsurface Flow Module (Comsol 2012c).
- Structural Mechanics Module (Comsol 2012d).

The near-field hydrology models require input from the regional hydrogeology models that are calculated using the DarcyTools code. A dedicated interface has been programmed for this purpose, called iDC.

Comsol Multiphysics including its modules is a wide-spread commercial code belonging to category 3. The iDC code is a user programmed addition to commercial code and belongs to category 4a.

3.5.2 Suitability of the code

Comsol Multiphysics solves space and time dependent governing equations from a wide range of application areas, including fluid flow, heat transfer, mass transfer and chemical reactions, structural mechanics, and electromagnetics. In the SR-PSU, Comsol has been used to solve the equations describing saturated porous media flow and linear structural mechanics. These tasks are described in detail in Abarca et al. (2013, 2014) and in von Schenck and Bultmark (2014). The equations solved and the numerical methods used are described in the software documentation (Comsol 2012a, b, c, d).

3.5.3 Usage of the code

Documentation of Comsol Multiphysics and its modules is provided by the code developer, Comsol AB. The developer provides technical support and software training, as well as an on-line forum for the Multiphysics modelling community.

3.5.4 Development process and verification

Comsol Multiphysics is a wide spread commercial code, supported by the QA processes of the code developer, Comsol AB. The user-programmed iDC code has been tested and verified, as described in Abarca et al. (2013).

3.5.5 Handling of input data, computational results and scripts

The models for the near-field hydrology (Abarca et al. 2013) extract pressure and flux boundary conditions as well as rock permeability fields from the regional hydrogeology models. Model files from the Darcy Tools software serve as input in this regard. Material properties describing repository components, such as concrete and bentonite, are available from the **Data report** and are assigned directly as numerical values in the models.

The structural mechanics modelling performed to assess how swelling waste may affect concrete barriers (von Schenck and Bultmark 2014) in the repository takes literature data on swelling waste as input parameters (**Data report**).

Model files, model output, and auxiliary code such as the iDC are stored on a backed up SKB server. The version management system Subversion SVN (Küng and Onken 2009) is used to keep track of changes.

3.5.6 Rationales for using the code in the assessment

Comsol Multiphysics is used in SR-PSU assessment for several reasons. One of the main benefits of the code is the ability to solve space and time dependent models of coupled processes in a flexible way. This means that existing models can readily be extended without restarting the modelling process or changing the simulation tool. For instance, near-field flow models can serve as basis for reactive transport modelling in further assessment tasks. Furthermore, Comsol is a wide-spread commercial code, granting vendor QA, technical support, and documentation. The software offers interfaces to CAD software such that repository design geometries can be used directly in the technical analysis. Comsol Multiphysics also provides interfacing to technical computing software, and script programming in Java. This allows for user defined extensions of the standard functionality as well as the opportunity to couple Comsol to other modelling tools used in the assessment.

3.6 DarcyTools

3.6.1 Introduction

DarcyTools computer code is used to simulate 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 top of the rock.

It is a general code for this class of problems, but was developed for the analysis of nuclear waste repositories.

A number of novel features are introduced in DarcyTools. The most fundamental is perhaps the method used to generate grid properties (DarcyTools is a continuum porous-media code), which allows a fracture network to be defined with specific properties assigned to each fracture. This network is represented "directly" in the computational grid. The method is believed to result in accurate anisotropy and connectivity properties. Another key feature is the grid system; an unstructured Cartesian grid is used in DarcyTools v3.4, which accurately represents objects that are read into the code as CAD-files.

DarcyTools is developed collaboratively by SKB, CFE AB (Computer-aided Fluid Engineering AB) and MFRDC (Michel Ferry Research&Development Consulting), with SKB as the owner of the code. It is based on the solver MIGAL (Ferry 2002) and development work on DarcyTools initiated in early 2001. The initial code built upon earlier groundwater models developed by CFE AB. One example is the general purpose equation solver PHOENICS (Spalding 1981) used to predict the inflow to the Äspö HRL, prior to its construction (Svensson 1991). The first well documented version of DarcyTools was v2.1, which was released in 2004. Version 3.4 is currently in use and the documentation of this version is available in Svensson et al. (2010), Svensson (2010) and Svensson and Ferry (2010). Both Windows 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. The code was used in the performance assessment for SR-site (Forsmark and Laxemar), as described in Svensson and Follin (2010), Svensson and Rhén (2010) and Vidstrand et al. (2010a, b).

3.6.2 Suitability of the code

Due to the collaborative (SKB and CFE AB/MFRDC) development of DarcyTools, it was decided from the start that DarcyTools would 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 investigation or glaciation studies. It is beyond the scope of the present text to describe these features (see Svensson et al. 2010) but they include: DFN-generation, free surface algorithm, multirate diffusion model and coupled groundwater flow and salt transport. In addition to these useful features, a code needs to be efficient. The unstructured grid mentioned earlier in combination with the equation solver MIGAL (an unstructured multigrid solver) ensures that DarcyTools v3.4 is a state of the art code with respect to efficiency. These features make DarcyTools v3.4 a suitable code for a wide range of problems that need to be considered by SKB.

3.6.3 Usage of the code

Three main documents (Svensson et al. 2010, Svensson 2010, Svensson and Ferry 2010) describe the code and its use in detail. Recent real world applications, for example Follin et al. (2005), Svensson and Follin (2010), Svensson and Rhén (2010) and Vidstrand et al. (2010a, b), provide other valuable sources of information. The usage of the code in SR-PSU is described in Odén et al. (2014).

Svensson and Ferry (2010) is a User's Guide, which describes all the input parameters. These input parameters make up the 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 aspect of the code is the ability to monitor 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 v3.4 it is even possible to plot the distribution of variables in specified planes.

3.6.4 Development process and verification

Svensson (2010) describes the verification, validation and demonstration of Version 3.4. 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"). Therefore, a number of comparisons with field data are included. So far, no attempt has been made to show that DarcyTools conforms to any international QA standard.

3.6.5 Handling of input data, computational results and scripts

The DarcyTools model uses human readable text files both as inputs and outputs. Most of the input data are taken from the SFR Site descriptive model and the **Climate report**. Outputs are mainly to the local hydrological modelling, the surface hydrological modelling and the radionuclide transport. All inputs and outputs are detailed in the AMF (Appendix A).

The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.6.6 Rationales for using the code in the assessment

DarcyTools has been selected for use in the safety assessment PSU because it has been developed by CFE AB and MFRDC in cooperation with SKB especially for solving the problem at hand. The calculations have been performed by several consultants with assistance by the main developer of the code.

3.7 Ecolego

3.7.1 Introduction

Ecolego is a flexible software tool for modelling dynamic systems and performing deterministic or probabilistic simulations. Ecolego is used in SR-PSU for modelling and simulating the radionuclide transport in the nearfield, geosphere and biosphere. Ecolego has been developed by Facilia AB and was originally sponsored by the Swedish Radiation Safety Authority (SSM) and the Norwegian Radiation Protection Authority (NRPA). Ecolego is now a commercial software and is used by companies and institutions all over the world. The version used within the SR-PSU project is Ecolego 6.0. Since Ecolego is a commercial code with a large user-base it belongs to category 3.

Ecolego was used in the SR-Site safety assessment to calculate landscape dose factors in the biosphere calculations (SKB 2010b).

3.7.2 Suitability of the code

Ecolego has been designed to maximise transparency and flexibility, while at the same time offer powerful numerical solvers. Large models with many compartments, expressions, parameters and species are easily managed with the user interface. Ecolego also has many features for quality assurance, such as:

- An integrated radionuclide database.
- An integrated parameter database, as well as the possibility to set up an external (shared) parameter database.
- Sub-system library.
- Unit checking.
- Sub-version support.

Ecolego supports both deterministic and probabilistic simulations. Sensitivity analysis can be performed on probabilistic results. The mathematical models are described in detail in the **Radionuclide transport report** and in Saetre et al. (2013).

3.7.3 Usage of the code

Ecolego has a thorough web-based user guide (www.ecolego.facilia.se) which is continuously updated by the developer. The user guide provides sufficient guidance for the use of the code, with step by step tutorials for the novice user and also full description of all implemented methods and features. At the same web site, there is also access to other resources such as a forum for support, ideas, answers and community talk as well as an issue tracker to report bugs and request improvements.

The correct usage of the code is assured since Ecolego, in the SR-PSU project, is used in close collaboration with the developer of the code.

3.7.4 Development process and verification

Ecolego has been developed since 2002 and has been verified and validated through several comparisons with both analytical solutions as with benchmarks of other software such as Amber and Simulink (Maul et al. 2004). The Ecolego software is continuously tested using the unit testing methodology.

3.7.5 Handling of input data, computation results and scripts

After a simulation, an Ecolego model is saved together with its input data and the results as an assessment file. Each simulation performed for SR-PSU has been stored as an assessment file at SKB's subversion server.

Input data used for simulations are extracted (using java code) from data files stored at SKB subversion server and are stored within the Ecolego assessment file. Java code used to run assessments in batches are archived on Facilia's internal concurrent versioning system (CVS).

3.7.6 Rationales for using the code in the assessment

Ecolego is used in SR-PSU since the code is suitable for risk assessments of complex dynamic systems evolving over time with a large number of species. Ecolego has databases and other add-ons especially designed for the field of radiological risk assessment.

The models used for biosphere modelling in SR-PSU involve a large number of parameters and complex relationships between the inputs and the outputs. In addition, Ecolego enables simulation of large number of assessments.

3.8 LOVECLIM

3.8.1 Introduction

The LOVECLIM 1.2 (Driesschaert et al. 2007, Goosse et al. 2010) is a 3D coupled Earth system model of intermediate complexity (EMIC). It includes the dynamics of the atmosphere (ECBilt), ocean and sea-ice (CLIO) and vegetation (VECODE).

LOVECLIM was used in SR-PSU in combination with the CCSM4 Earth system model in order to assess the potential for cold climate conditions in Forsmark in the next 60,000 years, see the **Climate report.** The sensitivity to future atmospheric greenhouse gas concentrations and future variations in the incoming solar radiation due to orbital variations was also estimated in a series of sensitivity simulations. LOVECLIM has not been used in previous safety assessments.

The LOVECLIM code is a category 3 code, written in Fortran. The simulations were performed on the Ekman supercomputer at the Parallell Computing Centre (PDC) at the Royal institute of technology (KTH) in Stockholm.

3.8.2 Suitability of the code

The atmospheric component of LOVECLIM, ECBilt, is a quasi-geostrophic, T21 spectral model, with three vertical levels. Since its spectral resolution corresponds to a coarse horizontal resolution of ~$5.6° \times 5.6°$, its surface topography is simplified. Its parameterisation scheme allows for fast computing and includes a linear long-wave radiation scheme. ECBilt contains a full hydrological cycle, including a simple bucket model for soil moisture over continents, and computes synoptic variability associated with weather patterns.

The ocean and sea-ice component of LOVECLIM, CLIO, is a primitive-equation 3D, free-surface ocean general circulation model coupled to a thermo-dynamical and dynamical sea-ice model. CLIO has a realistic bathymetry described by a $3° \times 3°$ horizontal resolution and 20 vertical levels. In order to improve the agreement between observed precipitation and the amount calculated in ECBilt-CLIO, a negative precipitation-flux correction is applied over the Atlantic and Arctic Oceans (Goosse et al. 2010). This flux is reintroduced in the North Pacific.

The dynamical terrestrial vegetation component of LOVECLIM, VECODE, computes the surface fraction of each land grid cell covered by herbaceous plants, trees and desert fractions and is coupled to ECBilt through the surface albedo (Driesschaert 2005).

3.8.3 Usage of the code

In the SR-PSU assessment, the LOVECLIM code was used by scientists with experience in climate modelling and the simulated climate was compared with data provided by the model developers. The version used in SR-PSU is described in Goosse et al. (2010).

The air temperature at 2 meters height (T_{2m}) simulated by LOVECLIM was used as input to the permafrost model (see Section 3.11). In SR-PSU, spatial interpolation was combined with a bias correction to account for the lack of regional and local detail arising from the coarse horizontal resolution of the LOVECLIM output. The monthly mean Forsmark T_{2m} was obtained from LOVECLIM output using inverse distance weighting. Subsequently, a bias-correction was performed on the output data before it was used as input to the permafrost model. The bias was assessed from an ensemble of three simulations of the pre-industrial (1751–1850 AD) climate. Since there is no data from Forsmark for this period, station data from Uppsala, located about 64 km southeast of Forsmark, was used to determine the bias in simulated T_{2m} in the Forsmark region. The annual average bias is +2.3°C with a maximum of +4.4°C in March and a minimum of –0.2°C in September (Brandefelt et al. 2013). To account for the bias, the monthly mean bias was subtracted from the LOVECLIM simulated T_{2m} interpolated to Forsmark.

To assess the potential of permafrost in Forsmark in the next 60,000 years, the coldest climate conditions simulated with LOVECLIM were chosen to produce a reference permafrost model simulation. The monthly mean T_{2m} simulated with LOVECLIM for the period of low summer insolation at high northern latitudes at 54 ka AP assuming a low glacial atmospheric CO_2 concentration of 180 ppmv was thus used.

The potential for colder conditions than those simulated with LOVECLIM due to uncertainties in the simulated climate was assessed by identification and quantification of a number of sources of uncertainty. These include future glacier and ice-sheet growth, inter-model differences, internal variability and future atmospheric greenhouse gas concentrations, see the **Climate report**, Section 4.2.4. The combination of all these uncertainties results in a pessimistic estimate of the minimum T_{2m} that could occur in Forsmark in the next 60,000 years. The resulting minimum annual average T_{2m} is about 6°C lower than that simulated with LOVECLIM for the high northern latitude summer insolation minimum at 17 ka AP and around 12°C lower for the insolation minimum at 54 ka AP, see the **Climate report**, Section 4.2.4.

3.8.4 Development process and verification

The first two components of LOVECLIM, which were coupled at the end of the 1990s, were the atmospheric model ECBilt and the sea–ice–ocean model CLIO, forming ECBilt-CLIO2. These two components are still at present the core of LOVECLIM, but have been improved significantly compared to the original versions. The version of the code used for SR-PSU is described in Goosse et al. (2010).

LOVECLIM has been used in an extensive range of research projects. It was included in the Climate Modelling Intercomparison Project 5 (CMIP5; http://cmip-pcmdi.llnl.gov/cmip5/) in support of the fifth assessment report of the Intergovernmental Panel on Climate Change (IPCC 2013; www.ipcc.ch). It was also included in the Paleoclimate Modelling Intercomparison Project 3 (PMIP3; www.pmip3.lsce.fr).

LOVECLIM produces a reasonably realistic modern climate (Driesschaert 2005) and an LGM climate generally consistent with data. Nevertheless, in a control climate forced with pre-industrial boundary conditions, a systematic warm bias of the annual mean surface air temperatures of about 2°C compared to a 1971–2000 climatology is found in the model (Driesschaert 2005).

Equilibrium climate sensitivity (ECS) is defined as the global equilibrium surface-air-temperature change in response to instantaneous doubling of atmospheric CO_2 concentration. The ECS is 1.7°C for LOVECLIM (Driesschaert 2005), which is low as compared to the ECS of 2.0–4.5°C for the Atmosphere-Ocean General Circulation Models (AOGCMs) in IPCC AR4 (Randall et al. 2007) and the ECS of 2.1–4.7°C for the AOGCMs in CMIP5.

3.8.5 Handling of input data, computational results and scripts

A long list of input data and parameters are required by the LOVECLIM model. In the simulations performed for SR-PSU all input data and parameters were set at their default values (representing year 1850 AD) as given by the developers of the code, except for two sets of parameters. These are: obliquity, eccentricity and angle of vernal equinoxes (which determine the latitudinal and seasonal distribution of incoming solar radiation) and atmospheric greenhouse gas concentrations (carbon dioxide, methane and nitrous oxide)), which were changed in order to simulate future conditions. The model was run with constant forcing and boundary conditions in a number of sensitivity test. Further four simulations were performed with time varying latitudinal and seasonal distribution of incoming solar radiation. The time step used in the different model components varies from less than one day for the atmosphere, ocean and sea-ice to a year for the vegetation. Details of model setups and input data for individual SR-PSU simulations are found in the **Climate report**.

Output data on a list of atmospheric and oceanic variables, such as air temperature and ocean water temperature and salinity, are saved at monthly and annual resolution. These are given in a latitude-longitude grid. The atmospheric and vegetation variables are given on a Gaussian T21 grid, whereas the oceanic variables are given on a displaced pole grid.

Data were transferred between the LOVECLIM and permafrost simulations (see Section 3.8.4) by text files. The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.8.6 Rationales for using the code in the assessment

The LOVECLIM code was used for estimating the minimum near-surface air temperature in Forsmark over the next 60,000 years. The uncertainty in the results was estimated based on comparison to simulations with the Earth system model CCSM4 (see Section 3.4) and other published studies. The output data that was used in the permafrost modelling is described in Section 3.11. The code was selected for the SR-PSU safety assessment since it is one of the world-leaders in its field.

3.9 MIKE SHE

3.9.1 Introduction

The near surface hydrological and hydrogeological code MIKE SHE (Système Hydrologique Européen) is a commercial code developed by the Danish Hydraulic Institute (DHI). The code describes the main processes in the land phase of the hydrological cycle, from rainfall to river flow (Graham and Butts 2005). The model consists of five different compartments (Figure 3-1): saturated zone, unsaturated zone, overland flow, evapotranspiration and channel flow, that apply different water flow calculations. 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 2012 (DHI 2012) has been used within the SR-PSU modelling. The system is certified for Windows XP Professional Service Pack 3 (32 bit), Windows Vista Business Service Pack 2 (64 bit) and Windows 7 Professional Service Pack 1 (32 and 64 bit). In the SR-PSU modelling both the Windows XP and Windows 7 have been used. MIKE SHE was also used in the SR-Site safety assessment, where the 2009 version of the MIKE SHE model was used. The main difference between version 2012 and 2009 is the possibility to work with time varying properties. Time varying properties in the Overland flow and Saturated zone flow compartments enable the model to simulate ground- and surface water flow under periglacial conditions (Bosson et al. 2012, 2013).

MIKE SHE has been used in the hydrological and near surface hydrological modelling for SR-PSU. The Site Descriptive (SDM) MIKE SHE model (Bosson et al. 2008) and the MIKE SHE SR-Site model (Bosson et al. 2010) were used to develop the models of present and future conditions within SR-PSU. Different climate cases have been analysed, including the effect on the hydrology of shoreline displacement and the development of the landscape. Water balances and water fluxes within and between biosphere objects in the radionuclide transport model for the biosphere (Saetre et al. 2013) have been quantified by and extracted from the MIKE SHE model for present and future conditions. The MIKE SHE modelling is reported in Werner et al. (2013a) and in the **Biosphere synthesis report**. The MIKE SHE model is a category 3 code.

3.9.2 Suitability of the code

MIKE SHE is an advanced integrated hydrological system capable of simulating both surface water and groundwater with the same precision as models that focus on either one. The code 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.

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 via 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 throughout the simulation. Water exchange between M11 and MIKE SHE is further described in Gustafsson et al. (2009).

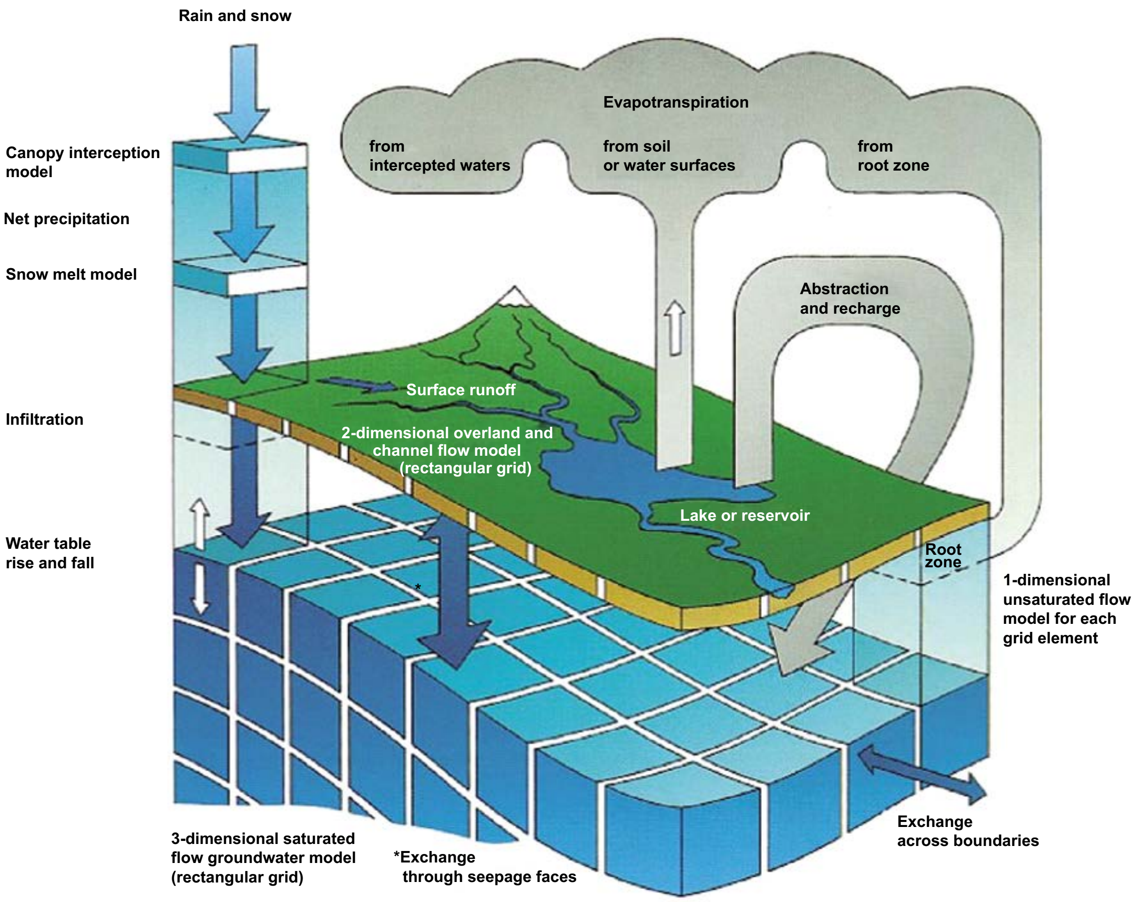

Figure 3-1. *The MIKE SHE model (Abbott et al. 1986).*

Based on the calculated flow field, particle tracking calculations (in the saturated zone) and advection-dispersion calculations can be performed (in all model compartments). Particle tracking calculations have been performed in the SR-PSU safety assessment.

There is a direct coupling between MIKE SHE and the GIS program ArcMap which is part of the ArcGIS framework, see Section 3.3. This is advantageous, 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.

3.9.3 Usage of the code

The MIKE SHE user manual (DHI 2012) consists of two documents;

- The MIKE SHE user guide:
  The document describes how to set up a model and how to process input and output data.
- The MIKE SHE reference guide:
  The document gives a detailed description of the individual tools and dialogs the user encounters when working with the MIKE SHE user interface. The document also includes detailed descriptions of the numeric engines and governing equations used in the MIKE SHE modelling system.

3.9.4 Development process and verification

The MIKE SHE model originates from the Système Hydrologique Européen (SHE) model, which became operational in 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 latest version of the model is MIKE SHE version 2014.

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 a high level of traceability for the input data to the model.

Many organisations have reviewed and evaluated the MIKE SHE code. Each review has had different objectives and has used different criteria in the review process. A number of references are available at the DHI website (www.dhigroup.com).

3.9.5 Handling of input data, computational results and scripts

Several modelling activities provided the various external input data and models required for the SR-PSU hydrological and near surface hydrogeological numerical modelling. The MIKE SHE SR-Site model was the starting point for all model cases simulated within the SR-PSU MIKE SHE modelling. The input data used in the SR-PSU MIKE SHE modelling is described in Werner et al. (2013b).

The MIKE SHE user manual is included as a pfd-file with the installation media. The manuals are not available in a printed version.

Input data are supplied to the code as text files, shape-files or ESRI-grid files. Result files are time series files, *.dfs0 or grid-files, *.dfs2 and *.dfs3. All dfs0-files, dfs2-files and dfs3-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 in an on-line User Manual.

All time series data from the site investigations, used as input data to the MIKE SHE model, are stored in the SKB Sicada database. Spatially distributed input data to the MIKE SHE model are stored in the SKB GIS database. Models and data from other scientific disciplines in the SR-PSU project that are used in the modelling are stored in the SKB Subversion system (svn\SFR\SR-PSU\Indata\parameter_indata).

The MIKE SHE model generates numerous result data files. For practical reasons the model result files cannot be uploaded on SKBDoc. A separate server at SKB has therefore been in use for storing the MIKE SHE results files. The server is accessible via G/SKB/modellering/ber, the server is only accessible for MIKE SHE users.

Details about all input data to the MIKE SHE SR-PSU model and references to specific data extractions from each database mentioned above are found in Werner et al. (2013a).

3.9.6 Rationales for using the code in the assessment

MIKE SHE is used in SR-PSU for hydrology and near surface hydrogeology calculations. MIKE SHE makes it possible to model the interactions between surface water, groundwater and evaporation processes and makes it possible to describe and understand the complexity of water flow in the surface system. The MIKE SHE model provides data on water fluxes in and between different compartments for the biosphere radionuclide transport model.

3.10 Numerical GIA model

3.10.1 Introduction

The GIA (Glacial Isostatic Adjustment) code is used to calculate the isostatic adjustment of the solid earth due to loading and unloading of 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 calculated.

In SR-PSU, the GIA code was used to determine relative sea-level and shoreline positions in the region of interest for the reconstruction of the last glacial cycle and for a future warm climate development. It is also used to carry out sensitivity tests regarding e.g. the influence of earth and ice model parameters on the output, see the **Climate report**.

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 and Mix 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). The GIA code was also used for the SAR-08 safety assessment for SFR (SKB 2008) and for the SR-Can (SKB 2006) and SR-Site (SKB 2010a) safety assessments for the final repository for spent nuclear fuel.

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 post-doctoral researchers working in either Milne's or Mitrovica's research groups. The version of the code used for SR-PSU, run on UNIX computing platform at the university of Durham, is the one described in Mitrovica and Milne (2003).

The GIA results obtained within SR-Site for the Forsmark site (SKB 2010a) were judged as adequate to use also for the SR-PSU safety assessment (**Climate report**). Therefore, no new GIA simulations were made for SR-PSU.

3.10.2 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 then 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 accounted for in the distribution of the load (Milne et al. 1999). Thirdly, changes to the rotational state of the Earth as a result of both surface and internal mass redistributions are considered (Mitrovica et al. 2005). And fourthly, the impact of lateral variations in Earth structure is taken into account when calculating the solid Earth response to loading. 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), the extension of the code to include lateral structure is described in Latychev et al. (2005).

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

3.10.3 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. In the SR-PSU project, the correct usage of the code was assured by working in close collaboration with the developer of the code. The version used in SR-PSU is described in Mitrovica and Milne (2003).

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-PSU 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.

3.10.4 Development process and verification

In the code development, the accuracy of the numerical schemes employed was tested through comparison with a number of analytical solutions.

A small number of research groups have developed their own sea-level codes based on the results presented in the papers referenced above. However, not all versions include the latest developments discussed in the most recent papers (e.g. Mitrovica and Milne 2003). The solid earth response to GIA-loading has been successfully benchmarked between several groups (http://www.fis.uniurb.it/spada/GIA_benchmark_results.html).

For SR-PSU, 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. A large portion of the GIA studies (SKB 2010a, Section 3.3.4, Whitehouse 2009, **Climate report**) was devoted to parameter selection (ice load history and Earth parameters) in order to make a detailed model validation through sensitivity studies and a dedicated case-study. Some of the simulations were evaluated against the present-day pattern of isostatic uplift over Scandinavia determined from GPS measurements (Lidberg 2007). The model validation showed, among other things, that 3D GIA simulations, with laterally varying properties of the Earth's crust, produce results more in line with observations than the 1D GIA simulations used in SR-PSU and SR-Site, see SKB (2010a, Section 3.3.4 ”A case study with a Fennoscandian 3D Earth structure”). The magnitude of the error introduced by using the 1D Earth model in SR-Site and SR-PSU instead of a 3D Earth structure is presented for Forsmark in SKB (2010a, Figure 3-49). In the **Climate report** (Section 2.2.7 "Handling of uncertainties in SR-PSU – Model simplification uncertainty") it is further described that the uncertainty in the results of the GIA simulations in some cases are large, up to several tens of metres. In order to strongly reduce this uncertainty in the description of the shoreline displacement for the coming few thousands of years, the data obtained from the GIA code was complemented by data extrapolated from observations for this initial future period (**Climate report**, Section 2.2.4 "Model studies – Modelling of future isostatic adjustment"). Hence, even though the model validation showed that the results from the GIA simulations in some cases contain large uncertainties, the results were used in such a way that this did not hamper the analysis in SR-PSU.

3.10.5 Handling of input data, computational results and scripts

Data were transferred between the ice sheet- (UMISM, see Section 3.12), GIA-, and permafrost simulations (see Section 3.11) by text or Excel-files. Figure 3-2 shows the input and output data shared between the three models.

3.10.6 Rationales for using the code in the assessment

The GIA code was used for simulating isostatic changes during the last glacial cycle and in a future warm climate for input to other SR-PSU safety assessment calculations. In addition a large number of sensitivity simulations on Earth and ice load models were performed. The code was selected for the SR-PSU safety assessment since it is one of the world-leaders in its field.

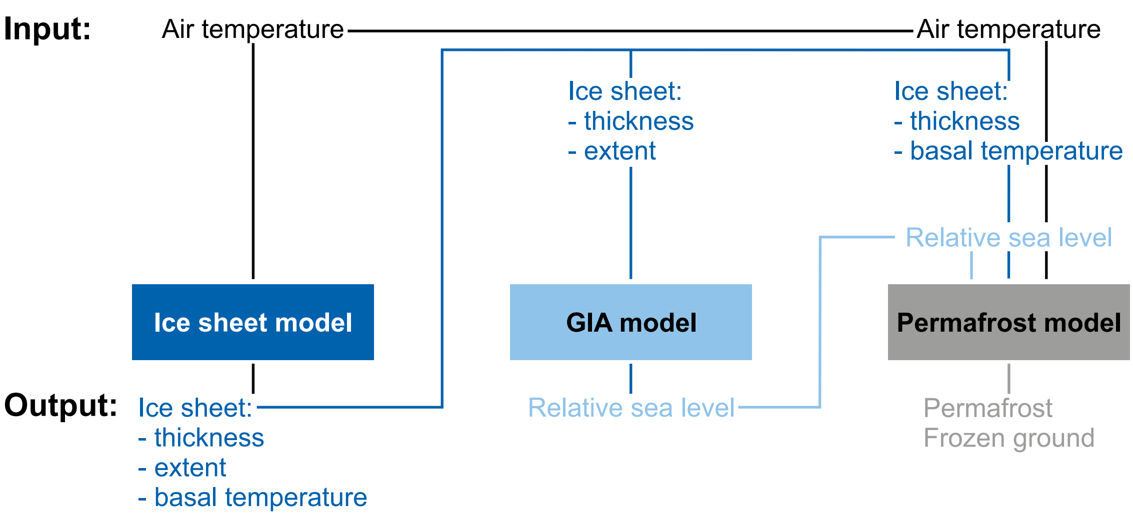

Figure 3-2. *Data transferred between the ice-sheet, GIA and permafrost simulations.*

3.11 Numerical permafrost model

3.11.1 Introduction

The numerical permafrost model code, written in Fortran, is used to calculate the development of permafrost and perennially frozen ground. Originally, the code was developed at the Helsinki University of Technology for soil freezing problems (Hartikainen 1994) being built on a general finite element solver code for non-linear non-stationary problems (Freund and Lempinen 1994).

The first version of the permafrost model code was written for the international project DECOVALEX III in order 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). Thereafter, the code was used in SR-Can (SKB 2006) to make a 1D reconstruction of the development of permafrost and perennially frozen ground at Forsmark during the last glaciation cycle and to perform sensitivity analyses on the important factors and parameters affecting the development of permafrost and frozen ground. For the SR-Site assessment, the code was updated to deal with spatially varying surface conditions and salt transport as well as to solve large systems of equations. The second version of the code was then used to investigate and demonstrate effects of multidimensional features of surface and subsurface conditions on the occurrence, development and distribution of permafrost and perennially frozen ground in a 2D vertical cross-section at Forsmark (Hartikainen et al. 2010). The study included features such as varying climate conditions, water bodies and topography, lateral variations in physical properties and heat generation from the spent fuel as well as effects of the phase change of saline water, groundwater flow and salt transport. These results, obtained with this second version of the code, are also used in SR-PSU for the reconstruction of the last glacial cycle climate at Forsmark (**Climate report**).

The code was further updated for SR-PSU to include seasonal freezing and thawing of the ground (Brandefelt et al. 2013). This third version of the code was used to investigate the potential for permafrost in the next 60,000 years in Forsmark (**Climate report**). Further, the sensitivity of the results to the improvements made in this third version as compared to the second version (Hartikainen et al. 2010) of the permafrost model was investigated (**Climate report**). The code is classified as a category 4b code. The permafrost model was run at a computing platform at Aalto University, Finland.

3.11.2 Suitability of the code

The second and third versions of the code solve the equations of energy balance and mass balance of groundwater, ice and salts together with the generalised Clausius–Clapeyron equation of the phase change between water and ice, the Darcy equation of groundwater flow and the equation of non-Fickian salt diffusion (Hartikainen et al. 2010, Brandefelt et al. 2013). The model considers the ground as a saline water saturated porous medium, and includes a description of the following physical processes:

- Heat and mass transfer in freezing and thawing ground.
- phase change of groundwater being affected by groundwater pressure and salt concentration.
- Exclusion of salt during freezing.
- Density dependent groundwater flow in unfrozen and partially frozen ground.

Anisotropies of material properties such as permeability and thermal conductivity are allowed. Information on surface conditions including air temperature, ice-sheet thickness, basal temperature, shoreline migration, and vegetation are given as time varying boundary conditions.

The code is based on the finite element method and implicit time integration schemes, and solves the above-mentioned coupled nonlinear partial differential equations using a consistent regularisation technique for discontinuities due to phase changes and the Newton–Raphson method for the nonlinear problem (Mikkola and Hartikainen 2002), and the preconditioned stabilised bi-conjugate gradient algorithm (van der Vorst 1992) for the system of linearised equations.

Prior to the SR-Site project, the code had been used to investigate soil freezing problems (Hartikainen and Mikkola 1997, 2006, Mikkola and Hartikainen 2001, 2002), and the development of permafrost and perennially frozen ground (Hartikainen 2004, 2006, Chan et al. 2005, SKB 2006).

A 3D version of the model has also been developed and used for simulations of permafrost and frozen ground at the Olkiluoto site in Finland (Hartikainen 2013).

3.11.3 Usage of the code

Description of the first version of the code is given in Freund and Lempinen (1994) and in Hartikainen (1994, 2004), while the model settings for the second version of the code, as well as SR-Site input and output data to the model, are described in Hartikainen et al. (2010). The model settings for the third version of the code, as well as SR-PSU input and output data to the model, are described in Brandefelt et al. (2013).

3.11.4 Development process and verification

The model development and verification for the second version of the code as well as the consistency of results between the second and first version of the code can be found in Hartikainen et al. (2010).

A validation of the second version of the numerical permafrost model was presented in Hartikainen et al. (2010, Section 3.6). The model was verified concerning i) density driven groundwater flow (see Section 3.6.1 "The Elder problem" and Section 3.6.2 "Salt fingering"), ii) the effect of pressure and salinity on the freezing temperature of water (Section 3.6.3 "Freezing point of saline water"), and iii) freeze-out of salt and salt transport in partially frozen soil (Section 3.6.4 "Uniaxial freezing").

The validation of density driven groundwater flow showed that the model gave somewhat faster development of the salinity concentration compared to the benchmark model used. The results further showed that the permafrost model produces results in good agreement with experimental observations of gravitationally driven convection of salt. The validation of the effect of pressure and salinity on the freezing temperature showed that the model generates data in very good agreement with experimental reference data. The validation of salt freeze-out showed that the model produces data in agreement with large-scale laboratory experiments.

The model development and verification for the third version of the code as well as the consistency of results between the third and second version of the code can be found in Brandefelt et al. (2013).

The validations described above show that the permafrost model is expected to provide results that fulfil the requirements of the SR-PSU safety assessment. Especially when also making use of the results and experience from the previously performed sensitivity analyses for the Forsmark site (Hartikainen et al. 2010).

3.11.5 Handling of input data, computational results and scripts

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. The data are transferred between the ice sheet- , GIA-, and permafrost simulations as shown in Figure 3-2. MATLAB and COMSOL are used to pre- and post-process the data.

The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.11.6 Rationales for using the code in the assessment

The code was selected for the SR-PSU safety assessment since it is one of the world-leaders in its field. The code was used in SR-PSU for simulations of freezing of saturated bedrock, for reconstructing last glacial cycle conditions and for assessment of the potential of permafrost in Forsmark in the next 60,000 years, as well as for a number of sensitivity tests.

3.12 Numerical ice sheet model (UMISM)

3.12.1 Introduction

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 the climate (advances and retreats resulting from changes in external forcing).

UMISM was used in SR-PSU for reconstructing the ice sheet for the last glacial cycle for the construction of the Weichselian glacial cycle climate case, and for input to simulations of other phenomena such as permafrost, isostatic changes, crustal stress, and ground water flow. The UMISM has previously been used for simulations of Fennoscandian ice sheets for various purposes, e.g. Fastook and Holmlund (1994), Holmlund and Fastook (1995), Näslund et al. (2003) and in SKB safety assessments (SKB 2006, 2008, 2010a).

The UMISM finite-element code (Fortran) has been developed by Prof. J. Fastook, at the School of Computing and Information Science at University of Maine, U.S.A., (e.g. Fastook and Chapman 1989, Fastook 1990, 1994, Fastook and Holmlund 1994, Fastook and Prentice 1994, Johnson 1994). In SR-PSU, the version of UMISM as of October 2004/April 2005 was used. The code is classified as a category 4b code.

The ice sheet model results obtained within SR-Site for the Forsmark site (SKB 2010a) were judged as adequate to use also for the SR-PSU safety assessment (**Climate report**). Therefore, no new ice sheet simulations were made for SR-PSU.

3.12.2 Suitability of the code

The climate input, forcing the ice sheet evolution, is the mean annual air temperature at sea level, and its variation over time and space. The ice sheet 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 lapse-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. If climate forcing so allows, 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.

3.12.3 Usage of the code

In the SR-PSU ice sheet reconstruction, input parameters to the model are; 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 this simulation, the code simulates the development of the Weichselian ice sheet for 120,000 years with 5 year time steps. For each time step, output data calculated for each grid cell and grid node are, for example, 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, e.g., ASCII format or NetCDF format.

Descriptions of model setups, as well as input data to the model, for SR-PSU simulations are found in the **Climate report,** Section 2.3.4. The close collaboration with the developer of the code assures the correct usage of the code in SR-PSU.

3.12.4 Development process and verification

UMISM was part of the EISMINT (European Ice Sheet Modelling Initiative) model intercomparison experiment and its output was in agreement with many other major thermo-dynamic ice sheet models, see Huybrechts et al. (1996) and Payne et al. (2000). The uncertainties associated with the model are presented in the **Climate report** (Section 2.3.7 – "Handling of uncertainties in SR-PSU – Model simplification uncertainty").

In the reconstruction of the Weichselian climate scenario, the ice sheet model was capable of producing a general development of the ice sheet in agreement with the overall Weichselian glacial history as known from studies of Quaternary geology and glacial morphology (**Climate report**, Section 3.2.1). For instance, the ice sheet model produced an ice configuration with very restricted ice coverage over Fennoscandia during the Mid-Weichselian period Marine Isotope Stage 3 (MIS3). Although this view was not generally accepted at the time when the simulations were performed (2005), studies of Fennoscandian Quaternary geology have showed that it was correct, see the **Climate report** (Section 3.2.1) and references therein. In addition, the ice sheet model yields results in broad agreement with Weichselian reconstructions based on completely different, Glacial Isostatic Adjustment (GIA) driven, methods (Schmidt et al. 2013, 2014). All this together shows that UMISM is expected to produce results that fulfil the requirements of the SR-PSU safety assessment.

3.12.5 Handling of input data, computational results and scripts

The code was adapted to meet specific requirements during the modelling 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-PSU activities, such as the permafrost modelling (Hartikainen et al. 2010, **Climate report**, Section 2.1.4), GIA modelling (**Climate report**, Section 2.2.4) and for modelling of crustal stresses (Lund et al. 2009). How data is transferred between the ice sheet (UMISM), GIA, and permafrost simulations is shown in Figure 3-2.

Data were transferred from the UMISM model to other SR-PSU activities in NetCDF files, ASCII files and Excel spread sheets.

3.12.6 Rationales for using the code in the assessment

The UMISM code was selected for the SR-PSU safety assessment since a very large number of simulations of the Fennoscandian ice sheet have been carried out with the UMISM model over the years. This has resulted in considerable experience and understanding 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 is the recognised 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.

3.13 PHAST

3.13.1 Introduction

PHAST v.1 (Parkhurst et al. 2004) simulates multi-component, reactive transport in saturated 1, 2 or 3D groundwater flow systems. PHAST is a versatile groundwater flow and solute transport simulator with the capability to model a wide range of equilibrium and kinetic geochemical reactions. The flow and the transport calculations use a modified version of HST3D (Kipp 1987, 1997) that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with PHREEQC (Parkhurst and Appelo 1999), which is embedded in PHAST.

PHAST has been used in the SR-PSU safety assessment for investigating the impact of fractures on the rate of concrete degradation in the barriers (Höglund 2014). PHAST has also been used as a numerical tool in a number of previous performance assessment studies for SKB (Arcos et al. 2006, Grandia et al. 2006, Luna et al. 2006, Domènech et al. 2006, Grandia et al. 2007, Sena et al. 2008, Sena et al. 2010).

The code is regularly updated, and both the code and its revision history are available at http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast/index.html. PHAST for Windows version 1.0.6.7671 was used for SR-PSU.

Since the code is open source, with a large user base and was not written exclusively for SKB projects, it is regarded as a category 3 code.

3.13.2 Suitability of the code

PHAST is a robust code with a large user base that is able to couple 1, 2 or 3D diffusive and advective transport with geochemical reactions. It is therefore ideal for investigating degradation processes in the concrete barriers of SFR, over time and space. In the SR-PSU application, PHAST calculated the water flow and resulting changes in the bulk composition of the pore water for each time-step and for each node. Then, PHREEQC was used to calculate the aqueous speciation, mineral dissolution/precipitation and ion exchange reactions. The calculated changes in the bulk composition of dissolved components and the mineral assembly were then returned to PHAST and the next time step was initiated. By using a sequential solution approach for flow, transport and reaction calculations, numerical solutions were obtained for each of the dependent variables. Finite differences techniques are used for the spatial and temporal discretisation of the flow and transport equations.

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. However, PHAST is restricted to a constant temperature and density, and is not suitable for some types of reactive transport modelling, in particular unsaturated zone flow, and transport of gas phases and non-aqueous liquid phases. More detailed information on the geochemical and transport equations that can be solved using this code can be obtained from the PHAST user's manual (Parkhurst et al. 2004)

3.13.3 Usage of the code

PHAST is explained in detail and example calculations are provided in the user's manual (Parkhurst et al. 2004). In addition to this, information, well documented examples and an active and interactive FAQ section are provided on the author's web site (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast/index.html).

3.13.4 Development process and verification

PHAST is an open source computer code developed by the United States Geological Survey. The code is widely used and its algorithm has been checked through several scientific publications and through the example files distributed with the computer program.

3.13.5 Handling of input data, computational results and scripts

Reactive-transport simulations with PHAST require three input files: a flow and transport data file, a chemistry data file, and a thermodynamic data base (see the **Input data report**). The flow and transport data file describes the grid, the transport parameters, including the time discretisation, and the boundary conditions. The chemistry data file describes the initial composition of the aqueous solutions in each volume (for each material), and the mineral precipitation/dissolution reactions to be modelled. All input data files are built with modular keyword data blocks and the spatial data are defined in 3D rectangular zones. All this information is easily introduced by means of .dat files.

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

3.13.6 Rationale for using the code in the assessment

The PHAST code was selected for solving 2D and 3D fluid flow and reactive transport problems (advection, diffusion and dispersion) under water saturated conditions in the concrete barriers. The program has been developed to a high standard, is ideal for addressing these problems and is wellsupported.

3.14 PHREEQC

3.14.1 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.

PHREEQC was used in SR-PSU for chemical speciation calculations over time and space and for 1-D transport calculations that account for speciation and changes in speciation. The primary objectives in SR-PSU have been to simulate the evolution of redox capacity (Eh) and pH in the SFR repository in different climatic and hydrological situations. It has been used previously in the SR-Can , SR-Site, and SAR-08 projects, and elsewhere, see Duro et al. (2006), Grivé et al. (2010) and Guimerà et al. (2006).

The PHREEQC code is open source and updated versions are released regularly. The code and revision history are available on http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/.

The pH reactive-transport simulations (Cronstrand 2014) were performed with PHREEQC 2.17 and BRGMs (Bureau de Recherches Géologiques et Minières) thermodynamic database Thermoddem (Blanc et al. 2007).

The redox evolution (Duro et al. 2012) calculations were preformed with the same version, but with a modified SKB thermodynamic database SKB_TDB_2009. The modifications are described further in Duro et al. (2012).

Since the code is open source with a large user base, and was not written exclusively for SKB projects, it is regarded as a category 3 code.

3.14.2 Suitability of the code

PHREEQC is a robust geochemical code that can be used to calculate saturation indices as well as the spatial and temporal distribution of aqueous species, including redox-sensitive elements. The code calculates the interactions of equilibrated aqueous solutions with minerals, gases, solid solutions, ion exchangers and sorption surfaces. It also has the capability to model kinetic reactions with rate equations given in the form of Basic statements. Additionally, it includes a 1D transport algorithm that allows dispersion, diffusion and various other parameters to be defined for dual porosity media.

More detailed information on the geochemical and transport equations that can be solved using this code can be obtained from the PHREEQC v.2 user's manual (Parkhurst and Appelo 1999).

Several limitations need to be considered. PHREEQC uses ion-association and Debye–Hückel expressions to account for the non-ideality of aqueous solutions (Parkhurst and Appelo 1999). This type of aqueous model is adequate at low ionic strength but may break down at higher ionic strengths (in the range of seawater). Another limitation of the aqueous model is the lack of internal consistency of the data in the databases.

3.14.3 Usage of the code

The PHREEQC v.2 user's manual (Parkhurst and Appelo 1999) describes the program in detail and examples are provided. The web pages of both authors (http://www.xs4all.nl/~appt/a&p/ and http://www.brr.cr.usgs.gov/projects/GWC_coupled/Phreeqc/) also contain information, well documented examples, and an active and interactive frequently asked questions (FAQ) section.

3.14.4 Development process and verification

PHREEQC is an open source code developed by the United States Geological Survey. The code is widely used and its algorithm has been checked in several scientific publications and through the example files distributed with the computer program. No modifications to the open source code has been reported in SR-PSU.

3.14.5 Handling of input data, computational results and scripts

All input and output files to PHREEQC are ASCII text files, which can be read and modified with standard spreadsheet tools such as Microsoft Excel. Two types of input files are needed: a thermodynamic data base and an input file describing the mineral precipitation/dissolution reactions to be modelled (either equilibrium or kinetically controlled), and mixing if included in the model. Diffusion processes can also be specified in this input file.

The **Input data report** describes the sources of the data used in the SR-PSU modelling by either detailing the location of the data files on the SKB server or providing a reference to the original report(s).

3.14.6 Rationales for using the code in the assessment

The PHREEQC code was selected for the SR-PSU safety assessment since it is able to perform 1D transport calculations in combination with speciation calculations using thermodynamic equilibrium data. The program is widely used, well suited to nuclear waste disposal scenarios and well supported.

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SKB's (Svensk Kärnbränslehantering AB) publications can be found at www.skb.se/publications.

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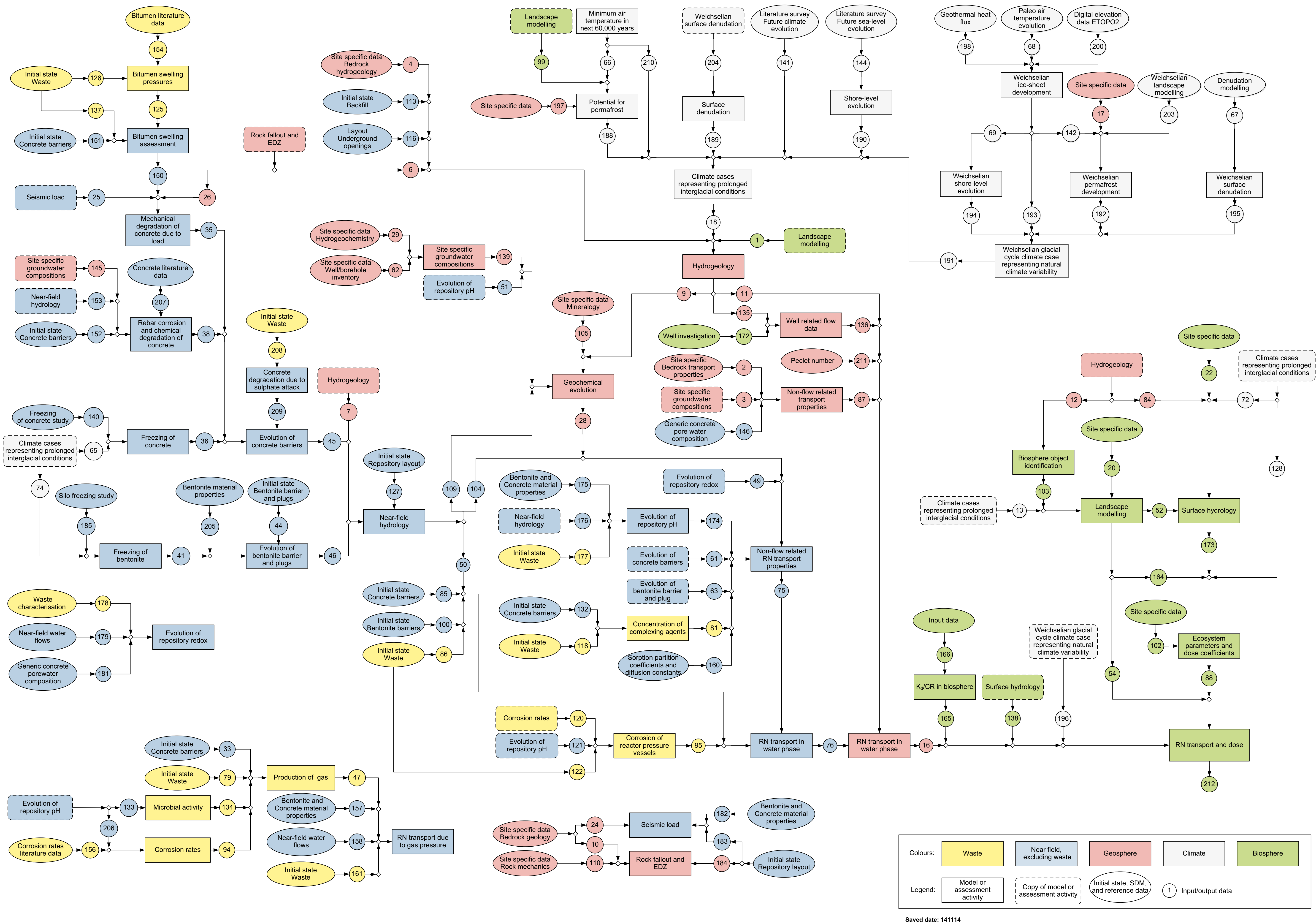
Bitumen literature data
Initial state Waste
Bitumen swelling pressures
Initial state Concrete barriers
Bitumen swelling assessment
Seismic load
Mechanical degradation of concrete due to load
Site specific groundwater compositions
Concrete literature data
Near-field hydrology
Initial state Concrete barriers
Rebar corrosion and chemical degradation of concrete
Freezing of concrete study
Climate cases representing prolonged interglacial conditions
Freezing of concrete
Silo freezing study
Freezing of bentonite
Bentonite material properties
Initial state Bentonite barrier and plugs
Evolution of bentonite barrier and plugs
Initial state Waste
Concrete degradation due to sulphate attack
Evolution of concrete barriers
Hydrogeology
Waste characterisation
Near-field water flows
Generic concrete porewater composition
Evolution of repository redox
Site specific data Bedrock hydrogeology
Initial state Backfill
Layout Underground openings
Rock fallout and EDZ
Site specific data Hydrogeochemistry
Site specific data Well/borehole inventory
Site specific groundwater compositions
Evolution of repository pH
Initial state Repository layout
Near-field hydrology
Initial state Concrete barriers
Initial state Bentonite barriers
Initial state Waste
Landscape modelling
Minimum air temperature in next 60,000 years
Site specific data
Potential for permafrost
Weichselian surface denudation
Surface denudation
Literature survey Future climate evolution
Literature survey Future sea-level evolution
Shore-level evolution
Climate cases representing prolonged interglacial conditions
Landscape modelling
Hydrogeology
Site specific data Mineralogy
Geochemical evolution
Bentonite and Concrete material properties
Near-field hydrology
Initial state Waste
Evolution of repository pH
Evolution of repository redox
Evolution of concrete barriers
Evolution of bentonite barrier and plug
Initial state Concrete barriers
Initial state Waste
Concentration of complexing agents
Sorption partition coefficients and diffusion constants
Non-flow related RN transport properties
Well investigation
Well related flow data
Site specific Bedrock transport properties
Site specific groundwater compositions
Generic concrete pore water composition
Peclet number
Non-flow related transport properties
Corrosion rates
Evolution of repository pH
Corrosion of reactor pressure vessels
RN transport in water phase
RN transport in water phase
Initial state Concrete barriers
Initial state Waste
Production of gas
Evolution of repository pH
Microbial activity
Corrosion rates literature data
Corrosion rates
Bentonite and Concrete material properties
Near-field water flows
Initial state Waste
RN transport due to gas pressure
Site specific data Bedrock geology
Site specific data Rock mechanics
Seismic load
Rock fallout and EDZ
Bentonite and Concrete material properties
Initial state Repository layout
Geothermal heat flux
Paleo air temperature evolution
Digital elevation data ETOPO2
Weichselian ice-sheet development
Site specific data
Weichselian landscape modelling
Denudation modelling
Weichselian shore-level evolution
Weichselian permafrost development
Weichselian surface denudation
Weichselian glacial cycle climate case representing natural climate variability
Hydrogeology
Site specific data
Climate cases representing prolonged interglacial conditions
Site specific data
Biosphere object identification
Climate cases representing prolonged interglacial conditions
Landscape modelling
Surface hydrology
Input data
K_d/CR in biosphere
Surface hydrology
Weichselian glacial cycle climate case representing natural climate variability
Site specific data
Ecosystem parameters and dose coefficients
RN transport and dose
Colours:
Waste
Near field, excluding waste
Geosphere
Climate
Biosphere
Legend:
Model or assessment activity
Copy of model or assessment activity
Initial state, SDM, and reference data
1 Input/output data
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