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Post-closure safety for the final repository for spent nuclear fuel at Forsmark

Model summary report, PSAR version

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Svensk Kärnbränslehantering AB

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Summary

This document is the model summary report for the PSAR for a final repository at the Forsmark site. In the report, the quality assurance (QA) measures conducted for assessment codes are presented together with the chosen QA methodology.

In a safety assessment project, a large number of numerical models are used to analyse the system and to show compliance to regulatory requirements. In order to better understand how the different models interact and how information are transferred between the different models Assessment Model Flowcharts, AMF's, are used. From these, different modelling tasks can be identified and the computer codes used.

As a large number of computer codes are used in the assessment and the complexity of these differs to a large extent. Some of the codes are commercial while others are developed especially for the assessment at hand. QA requirements must on the one hand take this diversity into account and on the other hand be specific. In the methodology section of the report, the following requirements are presented:

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

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

Subsequent to the methodology section, each assessment code is presented together with a discussion on how the requirements are met.

Contents

1 Introduction

This report summarises documentation of key models used in the assessment of post-closure safety in SKB's Preliminary Safety Assessment Report (PSAR) for a final repository for spent nuclear fuel at Forsmark. In order to start the construction of the final repository, SKB is required, under the Act on Nuclear Activities, to obtain an approval of the PSAR, see further Chapter 1 of the **Post-closure safety report**.[1] As described in Section 2.5.12 of the **Post-closure safety report**, the present report is one of 16 main references for the **Post-closure safety report** and is there referred to as the **Model summary report**.[2]

In the current chapter, the Model summary report is introduced. This is followed by a brief presentation of other documents within the PSAR Post-closure safety assessment and an outline of the current report.

1.1 Objectives and scope of the current report

The current report supports the **Post-closure safety report** and is an update of the SR-Site Model Summary Report (SKB 2010a) that supported SKB's license application submitted in 2011 (SKB 2011). The objective of the report is to give an overview of the modelling tasks and computer codes used in the PSAR Post-closure safety assessment, the quality assurance procedures and the documentation relating to the codes. More specifically, the report contains:

- Assessment model flow charts (AMF's) that describe the modelling tasks in the assessment and how the different modelling tasks are related.
- The principles behind the QA measures regarding the codes and the calculations.
- A brief presentation of each code used for modelling tasks identified in the AMF, with references to other documents that describe the mathematical model (the equations solved), verification measures, QA routines for input data handling and storage of results, QA routines for code development, version control, etc.

The aim is, however, not to give rationales for including a certain process in the modelling or to justify the selected input data. This is done in the three Process reports and a Data report, respectively.

1.1.1 Extent of update of the SR-Site Model Summary report

As mentioned above, the present report is an update of the SR-Site Model Summary Report (SKB 2010a). Much of the modelling tools and model results are unchanged since SR-Site. In these parts, the update is largely based on SKB's response (Hedin 2013) to a request from SSM for additional information regarding documentation and quality assurance of computer codes in the assessment. One new code, GRISLI (Section 3.10), used in the PSAR has been included. The analytical model for quantification of buffer erosion and sedimentation, and of canister corrosion (Section 3.3) has been updated with new features reflecting new knowledge that has emerged as regards buffer erosion and sedimentation since the SR-Site assessment. The introductory Chapters 1 and 2 have been updated to reflect the context of the PSAR. Assessment model flowcharts, Figure 2-1 and Figure 2-2 and associated tables Table 2-1 and Table 2-2, have been modified, mainly as a consequence of the previously described updates, and a few errors have been corrected.

[1] To improve readability, abbreviated names in bold font are used to refer to the PSAR **Post-closure safety report** and its main references, see further Section 1.2 and Table 1-1.

[2] The present report is published some time before the submission of the PSAR. In case the need for any changes of the contents of this report arises between its publication and the submission of the PSAR, a report of these changes will be provided in the PSAR.

1.2 Key reports in the assessment

Several of the steps carried out in the PSAR Post-closure safety assessment result in specific reports that are of central importance for the conclusions and analyses in the **Post-closure safety report**. These specific reports are referred to as main references. Besides the main references there are additional references, treating more narrow issues, supporting the **Post-closure safety report** and/or one or more of the main references. The report hierarchy is illustrated in Figure 1-1.

In addition to the Main and additional references, references are made to a variety of documents, articles and publications, either from SKB or from other organisations, or as part of the open literature.

1.3 Outline of the report

In the current chapter, the objective of the report is presented. In Chapter 2, the basic ideas for this report and requirements on codes used for assessment calculations are presented. The different modelling tasks and flow of information can be identified in the Assessment Model Flow charts (AMFs).

While some of the modelling tasks identified in the AMFs are simple scoping calculations, others require complex computer codes. As it would be impractical to include all kinds of modelling tasks performed within the framework of the safety assessment and to apply the same QA requirements on all computer codes used for modelling, the codes are subdivided into categories on which the requirements are formulated differently. The methods used for distinguishing between the different categories of codes are presented in Chapter 2. The QA requirements on codes used for the calculation tasks are also described in Chapter 2 together with a template used when describing each code.

Finally, in Chapter 3, the different codes used for the assessment calculations are presented following the outline presented in Chapter 2. Modelling data used in the safety assessment are archived at SKB, see Table 1-2.

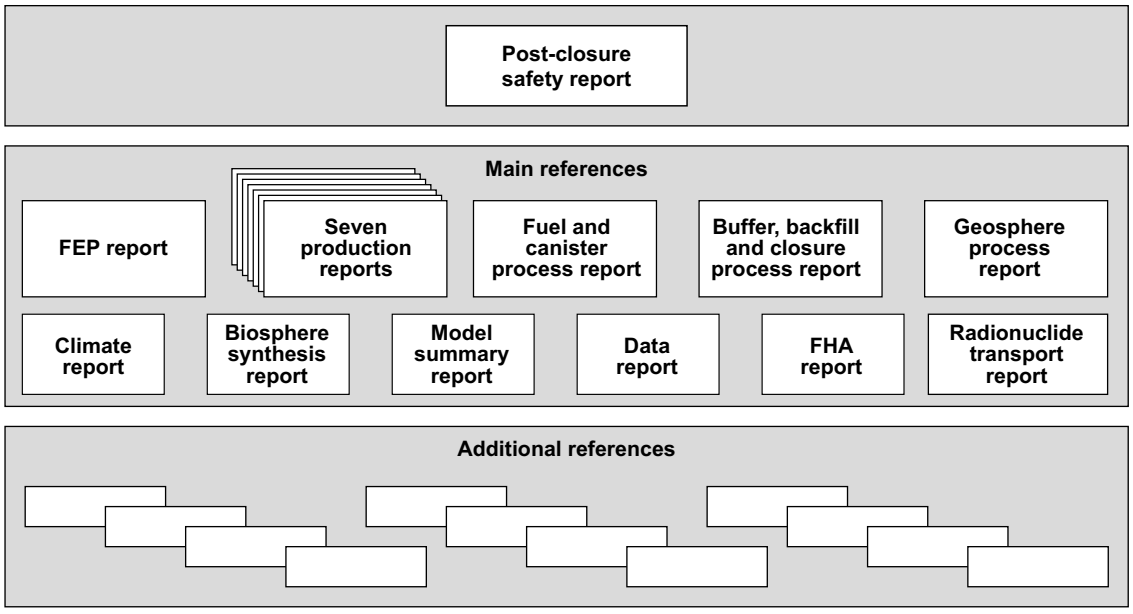

Figure 1-1. *The hierarchy of the main and additional references to the PSAR. The main references support the Post-closure safety report. The additional references may either support the Post-closure safety report directly or one of the main references.*

Table 1-1. Abbreviations and full references of SKB reports.

Abbreviation used when referenced in this report	Full reference, as given in the reference list
Buffer, backfill and closure process report	**Buffer, backfill and closure process report, 2022**. Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Buffer, backfill and closure process report, PSAR version. SKB TR-21-03, Svensk Kärnbränslehantering AB.
Buffer production report	**Buffer production report, 2022.** Produktionsrapport Buffert. SKBdoc 1392269 ver 5.0, Svensk Kärnbränslehantering AB. (In Swedish.) (Internal document.)
Canister production report	**Canister production report, 2022.** Produktionsrapport Kapsel. SKBdoc 1407944 ver 2.0, Svensk Kärnbränslehantering AB. (In Swedish.) (Internal document.)
Climate report	**Climate report, 2020.** Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Climate and climate-related issues, PSAR version. SKB TR-20-12, Svensk Kärnbränslehantering AB.
Data report	**Data report, 2022.** Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Data report, PSAR version. TR-21-06, Svensk Kärnbränslehantering AB.
FEP report	**FEP report, 2010.** FEP report for the safety assessment SR-Site. SKB TR-10-45, Svensk Kärnbränslehantering AB.
Fuel and canister process report	**Fuel and canister process report. 2022**. Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Fuel and canister process report, PSAR version. SKB TR-21-02, Svensk Kärnbränslehantering AB.
Geosphere process report	**Geosphere process report, 2022.** Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Geosphere process report, PSAR version. SKB TR-21-04, Svensk Kärnbränslehantering AB.
Post-closure safety report	**Post-closure safety report, 2022.** Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Main report, PSAR version. SKB TR-21-01, Svensk Kärnbränslehantering AB.
Radionuclide transport report	**Radionuclide transport report, 2022.** Post-closure safety for the final repository for spent nuclear fuel at Forsmark – Radionuclide transport report, PSAR version. SKB TR-21-07, Svensk Kärnbränslehantering AB.
Underground openings construction report	**Underground openings construction report.** Produktionsrapport Bergutrymmen, Svensk Kärnbränslehantering AB. (In Swedish.) (Internal document.) *In prep.*

Table 1-2. List of archived modelling data.

SKBdoc*, id, version	Title	Issued year
1256019 ver 1.0	Hydrogeological model data and results – Forsmark	2010
1258988 ver 2.0	Canister and buffer shear – App 10 I TR-10-34	2010
1929341 ver 1.0	Radionuclide transport calculations for the PSAR	2021
1262945 ver 2.0	Hydrogeochemistry: SR-Site and comparative analysis	2010
1927863 ver 1.0	Data used in the PSAR biosphere analysis for the final repository for spent nuclear fuel	2021
1264505 ver 1.0	Scripts and input data used in 3DEC modelling reported in TR-10-23	2010
1264508 ver 1.0	Scripts and input data used in 3DEC modelling reported in TR-08-11	2010
1264530 ver 1.0	Matlab scripts used in EFPC Development and Benchmarks (FPI chapter in MSR)	2010
1264531 ver 1.0	Matlab scripts used in EFPC/FPI modelling in SR-SITE (FPI chapter in MSR)	2010
1264532 ver 1.0	General Matlab codes used in EFPC/FPI modelling (FPI chapter in MSR)	2010
1265606 ver 1.0	CODE_BRIGHT Input files to the models used in SR-Site	2010
1265608 ver 1.0	Scripts and data used for Abaqus modelling of buffer in SR-Site	2010
1927770 ver 1.0	Models, input data and results for analytical erosion, sedimentation and corrosion calculations	2021
1927730 ver 1.0	Climate data used in the PSAR for the Spent nuclear fuel repository	2021
1265616 ver 2.0	Simple Functions calculations and data used in SR-Site	2010
1265618 ver 1.0	Scripts and data used for TOUGHREACT modelling in SR-Site	2010
1265689 ver 1.0	Oxygen ingress at Forsmark	2010
1265807 ver 1.0	PHAST data used for water saturated bentonite in SR-Site (TR-10-59)	2010
1266150 ver 1.0	Radionuclide transport calculations with MARFA	2010
1930115 ver 1.0	CODE_BRIGHT Input files to the models used in PSAR	2021
1930124 ver 1.0	Scripts and data used for Abaqus modelling of buffer in PSAR	2021

* Internal document

2 Quality assurance of modelling activities

In this chapter, methodology for quality assurance (QA) of modelling activities is discussed and requirements of relevance for QA of computer codes in the current safety assessment are presented.

Justification of the chosen conditions, including the chosen code, is given in modelling reports that describes the calculation. Motives for choosing a certain code are summarized in chapter 3 of the current report together with a decision to approve the use of the code in the assessment.

2.1 Assessment model flow chart and codes used in the assessment

Assessment Model Flow charts (AMFs) are used to illustrate how different modelling activities and assessments relate to each other and where modelling activities and data are reported. This includes what input the modelling activities use, what output the modelling activities generate and what data that are being transferred between modelling activities. In addition to the modelling activities included in the AMF, minor calculations are also performed, for instance when post-processing results or when preparing input data.

To describe the modelling activities in the current assessment, two AMFs have been prepeared, one representing the excavation/operation phase and initial temperate period, Figure 2-1 and one representing the period of periglacial and glacial conditions, Figure 2-2.

Computer codes used for the modelling activities presented in the AMF are presented in Table 2-1 and Table 2-2. As can be seen, a vast number of codes were used in the assessment. The complexity of the codes differs substantially and ranges from scripts for commercially available codes like MATLAB or Microsoft Excel to large programs (thousands of lines of code) written in programming languages like C++ and Fortran. The origin and user-base differ substantially, while some codes are commercial, have a large world-wide user base and can be regarded as well tested, others are developed within the safety assessment project and have a much smaller user-base. For codes developed within the safety assessment project, the source codes are generally available and can be reviewed. For commercial codes, this is usually not the case. Instead, verification tests and other quality assurance procedures performed by the developer have to be relied upon. A differentiated approach to quality assurance, with adaptations to the types of codes used in the assessment, is thus required.

For the current safety assessment, the following categories of computer codes have been identified:

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

4a. **Modified commercial or open source 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, the need for verification studies is larger than for codes in category 3. Using these codes for assessment calculations implies that the QA procedures used by the developer of the codes are accepted, but also that good developing practices are followed for the part of the code developed within the safety assessment.

4b. **Calculations performed with codes developed for the safety assessment**, frequently written in languages like C++ and Fortran. These codes are in general written with the safety assessment application in mind and have a considerably smaller user base than codes in category 3. The need for verification is thus larger for these codes.

There may be cases where it is not evident whether a code belongs to category 4a or to category 4b. Codes developed for the safety assessment may for instance contain routines from mathematical libraries (like ODE solvers etc.) which are well tested and have a large user base. However, the need for verification of the parts that have been added is the same for 4a and 4b.

In Table 2-1 and Table 2-2, modelling activities, computer codes and modelling reports are presented. Modelling reports are supporting documents for the safety assessment and are the main source of information on the modelling activity. Conditions, assumptions, results and conclusions are discussed and justified in modelling reports which are reviewed following normal routines. In addition to information in modelling reports, the current document addresses some other issues of relevance for QA of modelling activities, namely:

- If the code is suitable for its purpose.
- If the code can be properly used, i.e. is the code sufficiently documented.
- If the code development process has followed appropriate procedures and that the code produces accurate results.

In addition to the modelling activities, the AMF also contains information on what data that are transferred between the different modelling activities. In the current report, it is also relevant to include

- How results are transferred between different modelling activities and which results that are stored.

Below, these issues are linked to requirements and a template for reporting how each code relates to these principles is presented.

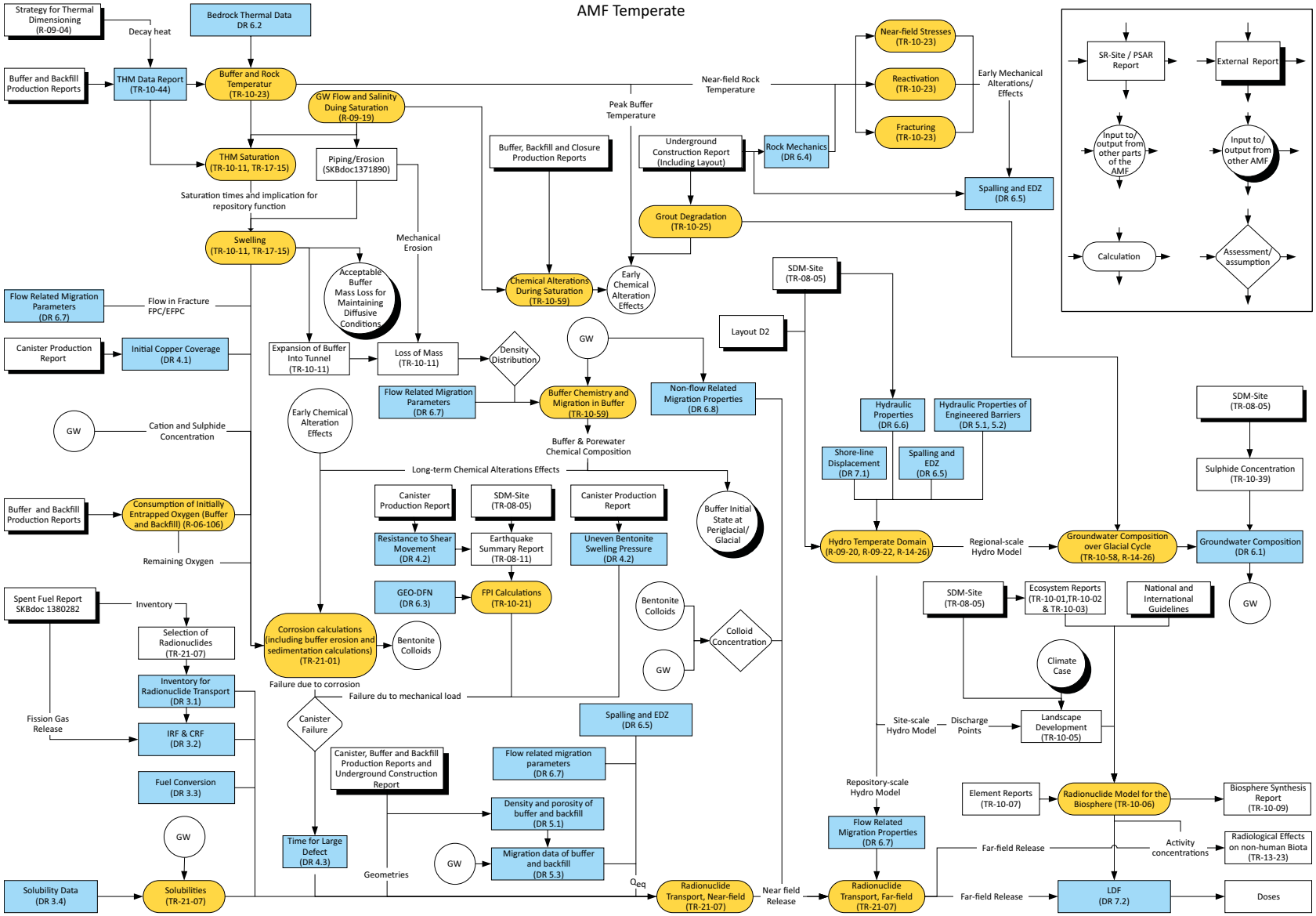

Figure 2-1. *The assessment model flow chart for the excavation/operation period and the initial temperate period after closure. In the AMF, modelling activities covered in the present report can be seen as yellow rounded rectangles. Input data and results (input data to other models) presented in the Data report (DR) appears as blue rectangles (with reference to the section in the Data report). Data in other reports are presented as rectangles.*

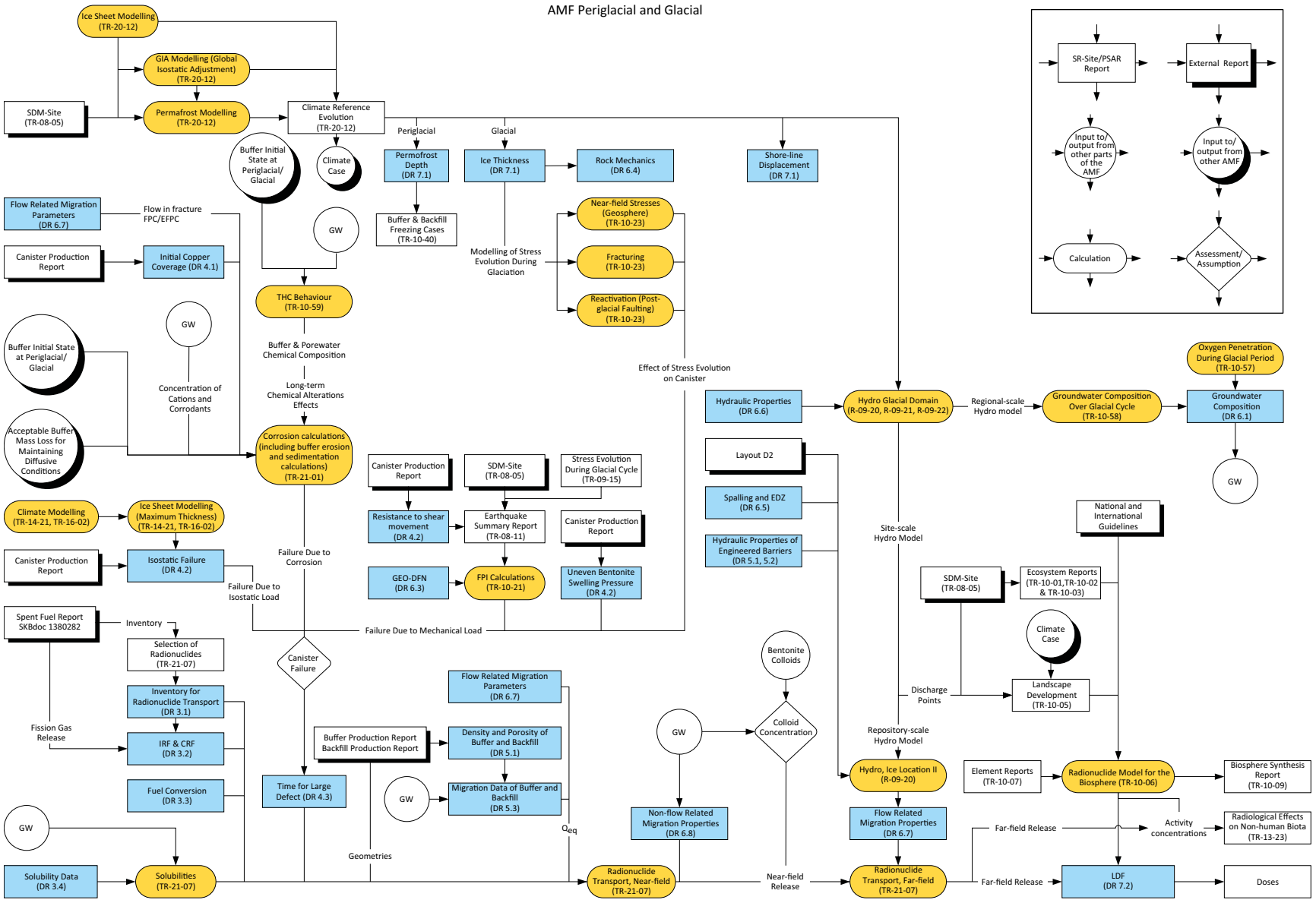

Figure 2-2. *The assessment model flow chart for periglacial and glacial conditions. In the AMF, modelling activities covered in the present report can be seen as yellow rounded rectangles. Input data and results (input data to other models) presented in the* ***Data report*** *(DR) appears as blue rectangles (with reference to the section in the* ***Data report****). Data in other reports are presented as rectangles.*

Table 2-1. Links between modelling activities in the AMF for excavation/operation and temperate periods and the computer codes used. The modelling activities in the left column correspond to yellow objects in Figure 2-1.

Modelling activity in AMF	Modelling report		Code used	Section
	In AMF	Reference		
Buffer and rock temperature	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Buffer chemistry and migration in buffer	TR-10-59	Sena et al. 2010a	PHAST, TOUGHREACT	3.19, 3.22
Corrosion calculations (including buffer erosion and sedimentation calculations)	TR-21-01	Post-closure safety report	Analytical expressions (Excel)	3.3
Chemical alterations during saturation (geosphere)	TR-10-59	Sena et al. 2010a	PHAST	3.19
Consumption of initially entrapped oxygen (buffer and backfill)	TR-06-106	Grandia et al. 2006	PHAST	3.19
FPI calculations (calculation of the occurrence of Full Perimeter Intersecting fractures in deposition tunnels)	TR-10-21	Munier 2010	FPI script in MATLAB	3.14
Fracturing (spalling)	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Groundwater composition over glacial cycle	TR-10-58 R-14-26	Salas et al. 2010 Joyce et al. 2015a	PHREEQC	3.20
Groundwater flow and salinity during saturation	R-09-19	Svensson and Follin 2010	DarcyTools	3.6
Grout degradation	TR-10-25	Grandia et al. 2010	CODE_BRIGHT	3.4
Hydro temperate domain	R-09-20 R-09-22 R-14-26	Joyce et al. 2010 Selroos and Follin 2010 Joyce et al. 2015a	ConnectFlow	3.5
Near-field stresses (geosphere)	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Radiological Effects on Non-human Biota	TR-13-23	Jaeschke et al. 2013	Erica	3.8
Radionuclide Model for the Biosphere	TR-10-06	Avila et al. 2010	Ecolego, MIKE_SHE, Pandora	3.7, 3.16, 3.15
Radionuclide transport, far-field	TR-21-07	Radionuclide transport report	FARF31, MARFA	3.9, 3.11
Radionuclide transport, near-field	TR-21-07	Radionuclide transport report	COMP23	3.13
Reactivation	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Solubilities	TR-21-07	Radionuclide transport report	Simple Functions	3.21
Swelling	TR-10-11 TR-17-15	Åkesson et al. 2010a Sellin et al. 2017	Abaqus, CODE_BRIGHT	3.2, 3.4
THM saturation (buffer and backfill)	TR-10-11 TR-17-15	Åkesson et al. 2010a Sellin et al. 2017	Abaqus	3.2

Table 2-2. Links between modelling activities in the AMF for periglacial and glacial periods and the computer codes used. The modelling activities in the left column correspond to yellow objects in Figure 2-2.

Modelling activity in AMF	Modelling report		Code used	Section
	In AMF	Reference		
Corrosion calculations (including buffer erosion and sedimentation calculations)	TR-21-01	Post-closure Safety report	Analytical expressions (Excel)	3.3
FPI calculations; calculation of the occurrence of Full Perimeter Intersecting fractures in deposition tunnels	TR-10-21	Munier 2010	FPI script in MATLAB	3.14
Fracturing	TR-10-23	Hökmark et al. 2010	3DEC	3.1
GIA modelling (Global Isostatic Adjustment)	TR-20-12	Climate report	Numerical GIA model	3.17
Groundwater composition over glacial cycle	TR-10-58	Salas et al. 2010	PHREEQC	3.20
Hydro, glacial domain	R-09-20 R-09-21 R-09-22	Joyce et al. 2010 Vidstrand et al. 2010a Selroos and Follin 2010	DarcyTools	3.6
Hydro, ice location II	R-09-20	Joyce et al. 2010	DarcyTools	3.6
Ice sheet modelling	TR-20-12	Climate report	UMISM	3.23
Ice sheet modelling (maximum thickness)	TR-14-21 TR-16-02	Colleoni et al. 2014 Quiquet et al. 2016	Grisli	3.10
Near-field stresses (geosphere)	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Oxygen penetration during glacial period	TR-10-57	Sidborn et al. 2010	PHREEQC, PHAST	3.20, 3.19
Permafrost modelling	TR-20-12	Climate report, details in Hartikainen et al. 2010	Numerical permafrost model	3.18
Radiological Effects on Non-human Biota	TR-13-23	Jaeschke et al. 2013	Erica	3.8
Radionuclide Model for the Biosphere	TR-10-06	Avila et al. 2010	Ecolego, MIKE_SHE, Pandora	3.7, 3.16, 3.15
Radionuclide transport far-field	TR-21-07	Radionuclide transport report	FARF31, MARFA	3.9, 3.11
Radionuclide transport near-field	TR-21-07	Radionuclide transport report	COMP23	3.13
Reactivation	TR-10-23	Hökmark et al. 2010	3DEC	3.1
Solubilities	TR-21-07	Radionuclide transport report	Simple functions	3.21
THC behaviour	TR-10-59	Sena et al. 2010a	PHAST	3.19

2.2 Template used for reporting the codes in Chapter 3

Based on the discussion in the previos section, four requirements regarding quality assurance of codes and calculation results apply:

1. It must be demonstrated that the code is suitable for its purpose. This is required for all categories defined above.
2. It must be demonstrated that the code is well documented so that it can be properly used. This is required for all categories defined above.
3. It must be demonstrated that the code development process has followed appropriate procedures and that the code produces accurate results. This requirement applies to codes in category 4 since these have been developed by the implementer. For codes in categories 1 to 3, the procedures of the developer are accepted.
4. It must be described how data are transferred between the different computational tasks. Note that this does not include a description on how data are handled internally by the model (covered in point 1 and 2 above and in documents where the calculations are presented), instead this section addresses data transfer between modelling activities. Due to the large number of modelling activities, it is possible that data is passed between activities in many different ways.

The requirements are further described below together with a template to be used when writing the code presentation for the model summary report. Of the six headings in the template, four relate directly to the basic requirements stated above.

2.2.1 Introduction

The code is briefly introduced and the categorisation according to the definition in Section 2.1 is given. This section should contain the following:

- A brief description of the modelling activity.
- 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 2.1, and a description of how the code has been developed.

This part may be written either by the assessment team or by subcontractors using the code.

2.2.2 Suitability of the code

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

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

This part may be written either by the assessment team or by subcontractors using the code.

2.2.3 Usage of the code

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

- A description of how the code is documented. Clearly, the format of the documentation may differ considerably between different codes and is hence not specified in this template. 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 assessment team or by subcontractors using the code.

2.2.4 Development process and verification

For codes that have been developed for the assessment 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 assessment team or by subcontractors using the code.

2.2.5 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 a version management system, i.e. Subversion SVN (Küng and Onken 2009) is used to keep track of changes.

This part may be written either by the assessment team or by subcontractors using the code.

2.2.6 Rationales 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 assessment team).

3 Description of the codes

This chapter describe codes used in PSAR modelling activities. Codes and associated modelling activities are presented in Table 3-1. Different versions have been used in the analysis which is a consequence of the long duration of the project. To require that only one version of a code is used in the analysis would either require that old calculations would have to be recalculated or that an updated version could not be used. Since every modelling report must justify the use of the selected code neither would increase the qualty of the assessment. The presentation of each code follows the outline presented in Section 2.2.

Table 3-1. Codes used in PSAR modelling activities.

Section	Code	Version(s) used
3.1	3DEC	4.1, 5
3.2	ABAQUS	6.5-3, 6.6-PR3, 6.7-5, 6.8-1, 6.8-3
3.3	Analytical model for quantification of buffer erosion and can-ister corrosion	0.7, 0.8, 0.9, 1.0, 2.0
3.4	CODE_BRIGHT	RetascoCodeBright based on CodeBright v.2), v. 2.2, v. 3beta (category 3), modified v. 3beta, v. 4
3.5	Connectflow	9.6
3.6	DarcyTools	3.4
3.7	Ecolego	4.0
3.8	ERICA	ERICA Tool v. November 2012
3.9	FARF31	1.2.1, SKBdoc 1260297 v 1.0
3.10	GRISLI	Versions as of June 2013 and September 2014
3.11	MARFA	3.2.2
3.12	Matlab	See sections 0–3.15
3.13	Matlab – Comp23	SKBdoc 1260297 v. 1.0
3.14	MATLAB-FPI	SKBdoc 1292573
3.15	MATLAB-Pandora	5172. 6745
3.16	MIKE SHE	MIKE SHE 2009
3.17	Numerical – GIA model	See Mitrovica and Milne 2003.
3.18	Numerical Permafrost model	Version 2
3.19	PHAST	Mainly 1.5.1, 2.10
3.20	PHREEQC	Mainly 2.10
3.21	Solubility model (Simple Functions)	SKBdoc 1265616 v.1.0, 2.0
3.22	TOUGHREACT	1.2
3.23	UMISM	Version from October 2004/April 2005

3.1 3DEC

3.1.1 Introduction

3DEC simulates the mechanical and thermo-mechanical response of discontinuous media subjected to either static or dynamic loading. 3DEC is a three-dimensional numerical program based on the distinct element method for discontinuum modelling (Itasca 2003, 2007). The program is based on the extensively tested formulation used by the 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 wastes. Both static and dynamic analyses for deep underground openings have been performed, see for instance (Stephansson et al. 1991, Sjöberg 1992, Senseny 1993). 3DEC has been used by SKB in earlier studies regarding thermo-mechanical effects on the bedrock around a deep repository (Hakami et al. 1998). Much of the rock mechanics analyses referred to in SR 97 were conducted using 3DEC. In 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), and for dynamic analyses of fracture shear displacements induced by post-glacial fault movements (Fälth and Hökmark 2006). In SR-Site 3DEC was used for similar analyses as those carried out in SR-Can:

- Static analyses of mechanical effects on rock and rock fractures within and around the repository. Effects caused by excavation of the repository openings, by pore pressures, by heat generation and glacial loads are considered. Effects of particular interest are creation of stress concentrations around the repository openings and fracture displacements that may change the hydraulic conditions. Both near-field and large-scale models are analysed (Hökmark et al. 2010). For these analyses, version 4.1 of 3DEC was used (Itasca 2007).
- Dynamic earthquake simulations are carried out to estimate the possible effects that post-glacial seismic events in pre-existing deformation zones may have on nearby fractures in terms of induced shear displacements (Fälth et al. 2010). For these analyses, version 3.0 of 3DEC was used (Itasca 2003).

After SR-Site, additional 3DEC (v. 5, Itasca 2013) simulations that confirm conclusions in SR-Site have been performed (Hökmark et al. 2019).

Since 3DEC is a wide-spread commercial code which allows the user to add functionality by use of the built-in programming language FISH, and since specifically developed FISH routines are integral parts of the SR-Site application calculations, 3DEC is regarded as a category 4a code.

3.1.2 Suitability of the code

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

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

The embedded programming language FISH is used for a number of tasks:

- The coordinates for each heat source are imported into 3DEC using FISH.
- It is used to reduce computer run time when analyzing thermo-mechanical static near-field models. 3DEC temperatures are calculated once for each set of models and then imported into different model versions using a specifically developed FISH routine.
- FISH is used for the development of a technique for defining circular-shaped fractures by assigning specific fracture material properties to selected parts of the discontinuities. This functionality is used in both the static analyses and in the dynamic earthquake simulations.
- In order to suppress irrelevant fracture shear movements in static thermo-mechanical models, a FISH routine is used to control fracture shear strength after each step-wise change of thermal stresses. It is also used to set pore pressures in the fractures.
- FISH is used to control boundary movements in the thermo-mechanical static near-field models.

In the earthquake simulations, FISH is used to control the initiation and propagation of fault rupture. Parameter values used in the SR-Site applications, i.e. values of rock mass and intact rock elastic parameters, values of fracture strength and fracture stiffness as well as values of rock thermal properties, are well within ranges covered by verified examples of analyses found in the extensive 3DEC literature (see e.g. Last and Harper 1990, Kulatilake et al. 1992, Cappa et al. 2006).

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 of the constitutive models that are implemented. A specific part of the documentation contains a description of the FISH language.

Text files containing all model data (geometries, material data, initial- and boundary conditions, solution strategies) are used as input to the code. In the input files, specific results to be monitored and recorded during the analysis can be specified. These results can be plotted or exported as text files. The FISH scripts are also written as text files. The scripts are activated by data calls in the input files.

3DEC has a plotting tool, which can be used for control of the model (geometry, application of boundary conditions etc) during model building. The plotting tool also has a wide range of possibilities for producing vector- and contour plots used during post processing of calculation results.

3.1.4 Development process and verification

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

The six different FISH routines used in the static (Hökmark et al. 2010) and dynamic (Fälth et al. 2010) 3DEC calculations that constitute background material for SR-Site are listed in Section 3.1.2). Two of these FISH routines were used to extend the functionality of 3DEC, i.e. to perform tasks that could not be performed with ordinary 3DEC commands at the time of the analysis. These two routines were used for:

- Definition of circular fractures.
- Initiation and control of fault rupture along a fault plane.

As stated in SKB (2010a), the development of all FISH routines was accompanied by tests to ensure that the routines work as intended. In addition, with regard to the two above-mentioned routines, their functionality is confirmed by results reported in Hökmark et al. (2010) and in Fälth et al. (2010). The functionality of the routine for the definition of circular fractures is confirmed by the contour diagrams in Hökmark et al. (2010, Figure 8-22). The diagrams show that shear motion occurs only

within the specified circular area. As regards the routine for initiation and control of fault rupture along a fault plane, Fälth et al. (2010, Figure 4-5) shows how the routine reduces the shear strength of the plane at different points at the time and at the pace as it is intended. In addition, this is demonstrated in Figure 5-2, Figure 5-3, and Figure 5-4 of Fälth et al. (2010), proving that the stress reduction routine, as intended and expected, results in a motion along the fault plane initiated in the predetermined hypocentre and propagating beyond the fault plane at the preselected rate.

The other four FISH routines were not intended to add any new functionality to 3DEC, but to streamline simulation work. For example, they were used to automate input and automate application of boundary conditions and properties of fracture minerals. As with all modeling work with 3DEC, regardless of whether a model is driven entirely by manually entered commands or, in whole or in part, using command scripts, it was subsequently checked that initial and boundary conditions were in accordance with the modeling task description. Therefore, there is no specific documentation of the checks made to ensure that automation as such works. In most cases these checks are trivial. For example, it is directly apparent if the heat sources in the thermomechanical calculations (canister positions with coordinates loaded from file using FISH scripts) are positioned as intended, i.e. in accordance with Layout D2 (Hökmarket al. 2010, Figures 5-11 and 5-12). Temperatures and temperature increments are calculated based on regular grids of point sources and with identical heat transport properties (Hökmark et al. 2010, Figure A1). Figure 3-1 below shows that the results from temperature import routine is accurate.

3.1.5 Handling of input data, computational results and scripts

The results from the static models analysed by Hökmark et al. (2010) were documented and evaluated within that study. They were used to make estimates of the potential for thermally induced spalling around the repository openings and of transmissivity changes in fractures and fracture zones. The text files containing all model input data and the corresponding FISH scripts are stored at Clay Technology's data server (administrativa dokument\Projekt\3DEC SR-Site\data) as well as at the record management system at SKB (SKBdoc 1264505, see Table 1-2).

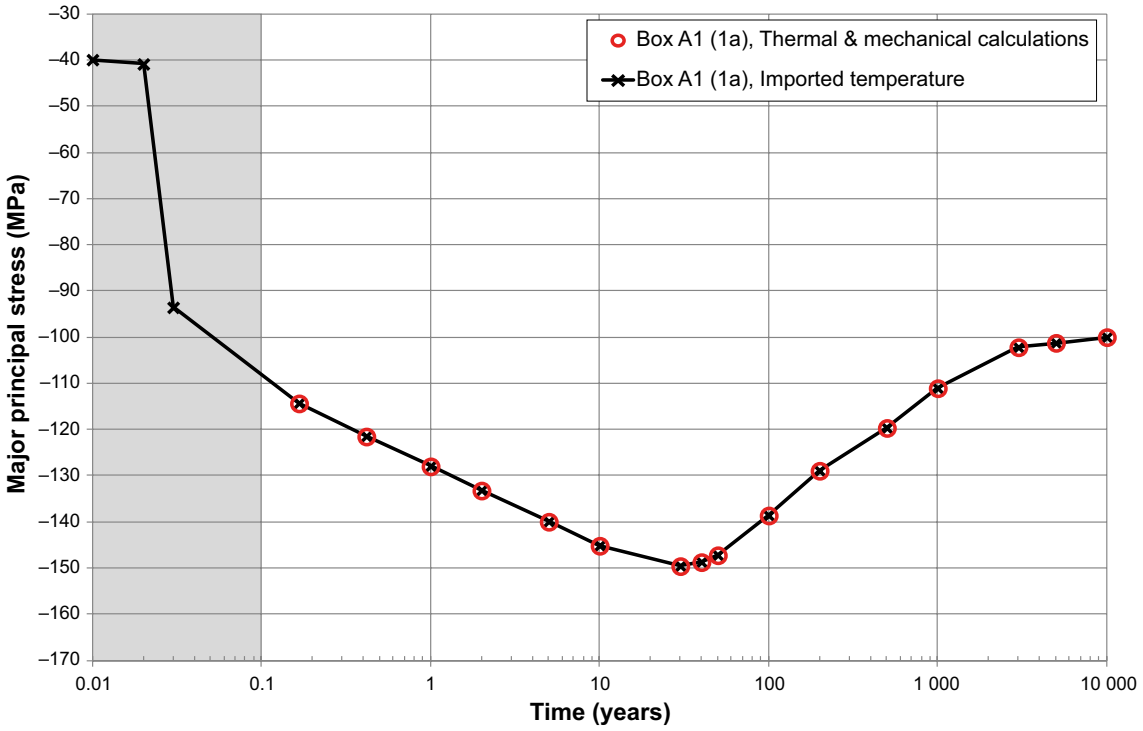

Figure 3-1. *Highest main stress at the canister height centre calculated using the temperature import routine and with direct temperature calculation (See Figure 9-7, left, in Hökmark et al. 2010).*

The results from the dynamic earthquake models analysed by Fälth et al. (2010) were documented and evaluated within that study where they were used for the development of schematic deposition rules. The text files containing all model input data and the corresponding FISH scripts are stored at Clay Technology's data server (administrativa dokument\Projekt\3DEC dynamik\data\Input files (Fälth et al. 2010)) as well as at the record management system at SKB (SKBdoc 1264508, see Table 1-2).

3.1.6 Rationales for using the code in the PSAR

The code 3DEC has been thoroughly tested and shown to be adequate for the intended purpose. Models and scripts have been successively developed and backward traceability is thereby warranted. The assessment team considers 3DEC being the code that best fulfil the purpose of the modelling and has therefore chosen to continue using 3DEC as the main tool both for static analyses and dynamic earthquake analyses.

3.2 Abaqus

3.2.1 Introduction

Abaqus is a suite of powerful engineering simulation programs, based on the finite element method, that can solve problems ranging from relatively simple linear analyses to the most challenging nonlinear simulations. Abaqus contains an extensive library of elements that can model virtually any geometry. It has an equally extensive list of material models that can simulate the behaviour of most typical engineering materials including metals, rubber, polymers, composites, reinforced concrete, crushable and resilient foams, and geotechnical materials such as soils and rock. Designed as a general-purpose simulation tool, Abaqus can be used to study more than just structural (stress/displacement) problems. It can simulate problems in such diverse areas as heat transfer, mass diffusion, thermal management of electrical components (coupled thermal-electrical analyses), acoustics, soil mechanics (coupled pore fluid-stress analyses), piezoelectric analysis, and fluid dynamics.

Abaqus offers a wide range of capabilities for simulation of linear and nonlinear applications. Problems with multiple components are modelled by associating the geometry defining each component with the appropriate material models and specifying component interactions. In a nonlinear analysis Abaqus automatically chooses appropriate load increments and convergence tolerances and continually adjusts them during the analysis to ensure that an accurate solution is obtained efficiently.

Interaction

Manufacturing processes, bolted assemblies, snap-fits, and impact events all involve interaction between contacting bodies. Understanding the behaviour of components when they come into contact is critical to designing better products. The Abaqus Unified FEA product suite provides comprehensive contact modelling capabilities such as the ability to model interactions between deformable bodies, rigid bodies, and self-contact.

The general contact capability in Abaqus automatically detects contact between different bodies with little need for user intervention. Solution accuracy is improved by eliminating the possibility of missed contact definitions. This powerful capability dramatically reduces the time needed to define contact for complex assemblies such as those found in automobiles, aircraft, consumer products, and portable electronics.

Abaqus/Standard

Abaqus/Standard is a general-purpose analysis product that can solve a wide range of linear and nonlinear problems involving the static, dynamic, thermal, and electrical response of components. Abaqus/Standard solves a system of equations implicitly at each solution "increment." In contrast, Abaqus/Explicit marches a solution forward through time in small time increments without solving a coupled system of equations at each increment (or even forming a global stiffness matrix).

Abaqus/Explicit

Abaqus/Explicit is a special-purpose analysis product that uses an explicit dynamic finite element formulation. It is suitable for modelling brief, transient dynamic events, such as impact and blast problems, and is also very efficient for highly nonlinear problems involving changing contact conditions, such as forming simulations.

Abaqus/CFD

Abaqus/CFD is a computational fluid dynamics analysis product. It can solve a broad class of incompressible flow problems including laminar and turbulent flow, thermal convective flow, and deforming mesh problems.

Abaqus/CAE

Abaqus/CAE (Complete Abaqus Environment) is an interactive, graphical environment for Abaqus. It allows models to be created quickly and easily by producing or importing the geometry of the structure to be analyzed and decomposing the geometry into meshable regions. Physical and material properties can be assigned to the geometry, together with loads and boundary conditions. Abaqus/CAE contains very powerful options to mesh the geometry and to verify the resulting analysis model. Once the model is complete, Abaqus/CAE can submit, monitor, and control the analysis jobs. The Visualization module can then be used to interpret the results.

Abaqus/Aqua

Abaqus/Aqua is a set of optional capabilities that can be added to Abaqus/Standard. It is intended for the simulation of offshore structures, such as oil platforms. Some of the optional capabilities include the effects of wave and wind loading and buoyancy.

Abaqus/Design

Abaqus/Design is a set of optional capabilities that can be added to Abaqus/Standard to perform design sensitivity calculations.

Geometry translators

Abaqus provides the following translators for converting geometry from third-party CAD systems to parts and assemblies for Abaqus/CAE:

- The CATIA V5 Associative Interface creates a link between CATIA V5 and Abaqus/CAE that allows you to transfer model data and propagate design changes from CATIA V5 to Abaqus/CAE.
- The SolidWorks Associative Interface creates a link between SolidWorks and Abaqus/CAE that allows you to transfer model data and propagate design changes from SolidWorks to Abaqus/CAE.
- The Pro/ENGINEER Associative Interface creates a link between Pro/ENGINEER and Abaqus/CAE that allows you to transfer model data and propagate design changes between Pro/ENGINEER and Abaqus/CAE.
- The Geometry Translator for CATIA V4 allows you to import the geometry of CATIA V4-format parts and assemblies directly into Abaqus/CAE.
- The Geometry Translator for I-DEAS converts parts and assemblies in I-DEAS to geometry files that can be imported by Abaqus/CAE.
- The Geometry Translator for Parasolid allows you to import the geometry of Parasolid-format parts and assemblies directly into Abaqus/CAE.

In addition, the NX Associative Interface creates a link between NX and Abaqus/CAE that allows you to transfer model data and propagate design changes between NX and Abaqus/CAE. The NX Associative Interface be purchased and downloaded from the Elysium web site.

Translator utilities

Abaqus provides the following translators for converting entities from third-party preprocessors to input for Abaqus analyses or for converting output from Abaqus analyses to entities for third-party postprocessors:

- Abaqus fromansys translates an ANSYS input file to an Abaqus input file.
- Abaqus fromnastran translates a Nastran bulk data file to an Abaqus input file.
- Abaqus frompamcrash translates a PAM-CRASH input file into an Abaqus input file.
- Abaqus fromradioss translates a RADIOSS input file into an Abaqus input file.
- Abaqus tonastran translates an Abaqus input file to Nastran bulk data file format.
- Abaqus toOutput2 translates an Abaqus output database file to theNastranOutput2 file format.
- Abaqus tozaero enables the exchange of aeroelastic data between Abaqus and ZAERO.

Abaqus is a widely spread commercial Finite element code developed and supported by Dassault Systèmes that has been available on the market for more than 40 years.

In the assessment, Abaqus has been used for a large range of applications, e.g. analyzing coupled thermo-hydro-mechanical (THM) problems or when simulating the response of the canister and buffer due to earthquake induced shear load. For the earthquake simulation, glacial load has also been included. These modelling activities have been presented in the following supporting documents to the assessment:

- Buffer homogenization (Åkesson et al. 2010a).
- Canister sinking (Åkesson et al. 2010a).
- Modelling and analysis of canister and buffer for earthquake induced rock shear and glacial load (Hernelind 2010).
- Heterogenous re-saturation of buffer (Sellin et al. 2017)
- Rock shear case with brittle shear propertiers (Sellin et al. 2017)

The buffer homogenisation modelling activities are part of the Canister Retrieval Test (CRT) within the Task Force for Engineered Barrier Systems (TF-EBS). The test was, in this context, used to study material models for unsaturated bentonite blocks and calculation techniques. Very similar results were reached with the Abaqus and the CODE_BRIGHT model, see Section 3.4 (Åkesson et al. 2010a) where a more detailed description of the modelling activity is given. Abaqus has been used for solving THM problems since SR97 (Börgesson and Hernelind 1999).

For modelling of canister sinking, Abaqus was used to simulate the vertical movement of a canister emplaced in a deposition hole due to creep. The equations to be solved and the material models used is presented in the modelling report (Åkesson et al. 2010a), corresponding problems were solved using Abaqus in SR-Can (Börgesson and Hernelind 2006a). In SR-Can, Abaqus was used to simulate Rock shear through a deposition hole (Börgesson et al. 2003, Börgesson and Hernelind 2006b). Abaqus is regarded to belong to category 3 and category 4a when user defined subroutines are used to extend the functionality.

Different versions of Abaqus (e.g 6.6-PR3, 6.7-5 and 6.8-1) has been used, mainly due to which latest version is available when the analyses are performed.

3.2.2 Suitability of the code

Abaqus is used for a number of tasks in the assessment, the equation solved are further described in each modelling report (Åkesson et al. 2010a, Hernelind 2010). The code is especially well suited for large, non-linear models including general interaction between different components involving several different fields such as displacement, temperature and pore pressure.

3.2.3 Usage of the code

Due to the large, world-wide user base there exists numerous user guides for the code, produced by the developer of the code and also by independent companies. The code is commonly used for different kind of mechanical modelling and there are common to find consultants specialised in using the code itself. Training classes are available at different levels both at universities and at private companies besides Dassault Systèmes.

3.2.4 Development process and validation

No dedicated verification or validation tests of the Abaqus code have been performed within the assessment project (the code has however been used to study material models in the Canister retrieval test with good results). A description of the QA procedures of the manufacturer of the code is available on their webpage as listed below.

The formal Quality Assurance Management System is the foundation of their efforts to deliver high quality products and services at an acceptable cost.

There are two principal reasons they impose strict quality assurance: customer satisfaction and product reputation. The approach to quality assurance meets the ISO 9001:2008 standard. The processes in their Quality Management System are designed to meet the requirements set forth by the International Organization for Standardization as defined within the ISO 9001:2008 Standard and also to facilitate customer compliance with US Nuclear Regulatory Commission's quality assurance requirements for software used for calculations associated with the design of nuclear power facilities in the USA.

Their Quality Management System is founded on a collection of well-documented processes that incorporate multiple checks and balances. The development process, for example, ensures that development is performed as a collaborative effort with proposal, design, code, and test review performed by a team representing developers, technical writers, the Quality Assurance group, management, and customers. Similarly, the bug management process calls for each bug to be reviewed by the Bug Manager, Quality Assurance Manager, and development group manager. Throughout the products' lifecycles, documented plans, formal signoffs, and dashboard-like status tracking facilitate establishing, communicating, and achieving clearly defined quality objectives.

There is no question that these efforts are resource intensive. Equally, there is no question that they are firmly committed to these processes, because the quality of their products and services is central to the long-term health of their relationships with their customers.

When user defined subroutines are used these have been verified by using simple test examples with known solutions (if possible) or by careful inspection of the obtained results.

3.2.5 Handling of input data, computational results and scripts

Buffer homogenisation and canister sinking

Input-files are stored on disk-systems at 5T Engineering and are archived at SKB's record management system (SKBdoc 1265608, see Table 1-2).

Modelling and analysis of canister and buffer for earthquake induced rock shear and glacial load

Scripts and input-files used for the analyses presented in Hernelind (2010) have been archived in SKB's record management system (SKBdoc 1258988, see Table 1-2).

Heterogenous re-saturation of buffer and Rock shear case with brittle shear propertiers

Scripts and input-files used for the analyses presented in Sellin et al. (2017) have been archived in SKB's record management system (SKBdoc 1930124, see Table 1-2).

3.2.6 Rationales for using the code in the PSAR

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

3.3 Analytical model for quantification of buffer erosion and sedimentation, and canister corrosion

3.3.1 Introduction

This model uses simple analytical expressions, derived and qualified elsewhere in the PSAR documentation, for calculations of the extent of buffer erosion and sedimentation, and canister corrosion (**Post-closure safety report**). The calculations are performed in Microsoft Excel.

The code is developed specifically for SKB and is classified as category 4b. A first version of the code was used in the safety assessment SR-Can (SKB 2006b) and a more developed version in the safety assessment SR-Site (SKB 2011). The present PSAR version has been further developed, mainly to encompass the new knowledge about the buffer erosion and sedimentation processes that has been gained since the SR-Site assessment.

3.3.2 Suitability of the code

The analytical model for quantification of buffer erosion and sedimentation, and canister corrosion is a direct implementation of the analytical expressions given in SKB (2010b) and references therein, and in Neretnieks et al. (2017). As shown in these references, the analytical expressions are derived for conditions and parameter ranges of relevance for the final repository. A significant development in this respect since the previous version is that buffer erosion is now modelled with groundwater cation concentration as a parameter. The analytical model is therefore judged to provide results relevant for the PSAR. Further justification of the expression for the corroded area under advective conditions used in the canister corrosion model is given in the response to a request for additional information on factors and processes that affect chemical erosion of the buffer, submitted to SSM on April 2, 2013, (Sellin 2013).

3.3.3 Usage of the code

The code is implemented as a Microsoft Excel-file (SKBdoc 1895159, see Table 1-2). Simple user instructions are provided in the file. Further explanations are provided in the code documentation (Hedin 2021).

3.3.4 Development process and verification

The mathematical models for buffer erosion and canister corrosion used in the PSAR are simple analytical expressions, described in SKB (2010b) and references therein, and in Neretnieks et al. (2017), which are readily implemented in this spreadsheet code.

A first version of the code was developed for the safety assessment SR-Can (SKB 2006b). The SR-Site version of the code was developed in several steps as documented in a history sheet in the Excel-file (SKBdoc 1895159, see Table 1-2). It has been verified that the code yields identical results as example calculations referred to in SKB (2010b).

SR-Site version

During SR-Site, three different versions (0.7, 0.8 and 0.9) were used. Version 0.8 was used for most of the final calculations in SR-Site. Earlier versions were used in preliminary calculations and in the development work. Version 0.7 was used for some of the sensitivity calculations presented in SKB (2010b). Version 0.9 was used for investigation of a particular detail for the case of diffusive transport

in the buffer, as also documented in SKB (2010b). The final SR-Site version 1.0 differs from v 0.8 only with respect to the comments in the Excel sheet, and in that some minor restructuring was done to enhance clarity and that some parts not used in SR-Site were deleted.

Documentation of the SR-Site version of the code including verifying tests is contained in SKBdoc 1396663 ver 1.0. That document describes version 1.0 of the code, with file name ErosionCorrosionModel_1_0.xlsx, stored under SKBdoc 1265612 in SKB's record management system SKBdoc.

PSAR version

The development of the SR-Site version into the PSAR version has mainly consisted of implementing features for calculating the extent of buffer erosion and sedimentation with the analytical expressions given in Neretnieks et al. (2017). Documentation of the PSAR version of the code including verifying tests is provided in Hedin (2021). That document describes version 2.0 of the code, with file name ErosionCorrosionModel_2_0.xlsx, stored under SKBdoc 1927770. A test input file with hydro data used for verification of version 2.0, named TestCaseHydro_2_0.xlsx, is stored under SKBdoc 1895160.

3.3.5 Handling of input data, computational results and scripts

Most input data are entered manually in the Excel-file and have default values that are write-locked in a specific version of the code. Hydrogeological input data (SKBdoc 1260297, 1256019, see Table 1-2) are provided in separate Excel files that are linked to the calculation file.

Key results of the extent of erosion and corrosion are obtained in a few output cells in the Excel file.

Results to be used as input to radionuclide transport calculations are automatically generated in a dedicated sheet, on a format suitable for that purpose. These data are stored in SKBdoc 1927770 (see Table 1-2).

The code is basically run in a single realisation mode. An Excel script (macro) is available to automatically run a number of realisations of a particular hydrogeological model. The Excel add-in @Risk is then used in combination with the script.

3.3.6 Rationales for using the code in the assessment

The code is tailor made for the needs in the PSAR. It has been developed and is used by members of the PSAR project.

3.4 CODE_BRIGHT

3.4.1 Introduction

In the safety assessment, CODE_BRIGHT (COupled DEformation BRIne, Gas and Heat Transport) is utilized for solving coupled thermo-hydro-mechanical (THM) problems in geological media. A large part of the TH, HM and THM simulations presented in Åkesson et al. (2010a) has been produced using CODE_BRIGHT. Some examples from Åkesson et al. (2010a) where CODE_BRIGHT is used are: Backfill saturation (H), Buffer saturation (TH), Buffer homogenization (THM), Backfill homogenization (HM) and Tunnel plug saturation (H). An analysis of the distribution of saturation times in the Forsmark repository (TH) was presented in Sellin et al. (2017). In addition, CODE_BRIGHT has been used in model calulations of grout degradation (Grandia et al. 2010).

In the SR-Can safety assessment, CODE_BRIGHT was used for investigating the influence of trapped air in the backfill (Börgesson et al. 2006). For references to other work concerning radioactive waste disposal where CODE_BRIGHT has been used (see CODE_BRIGHT v3 Validation document 2009). CODE_BRIGHT has been extensively verified and validated in international benchmark exercises, documented in CODE_BRIGHT v3 Validation document (2009), and has been applied to the analysis of different geoenvironmental schemes, waste disposal designs and geotechnical problems involving saturated/unsaturated soil behaviour.

CODE_BRIGHT is a Fortran code. Four different versions of the code, running on Windows platforms, have been used:

- Version 2.2 (category 3).
- Version 3beta (category 3).
- Version 3beta with modification 1 (category 4a).
- Version 3beta with modifications 1 and 2 (category 4a).
- Version 4 (category 3).

The unmodified code versions belong to category 3, whereas the modified code versions belong to category 4a. The modifications concern one of the mechanical constitutive laws, based on the Barcelona Basic Model (BBM).

In modification 1 the swelling modulus κ_s of BBM is made dependent on the void ratio by using experimental swelling pressure curves (see Åkesson et al. (2010a, Appendix C). Modification 2 consists of incorporation of a varying critical state line slope parameter M that is governed by an experimentally motivated deviatoric failure stress curve (see Åkesson et al. (2010a, Appendix D).

Research and development of the code is supported by the UPC (Technical University of Catalonia) and CIMNE (International Center for Numerical Methods in Engineering at UPC). A consortium of international companies contributes financially to these developments and checks the efficiency and quality of the resulting software. The consortium also provides a valuable link with geoenvironmental and geotechnical engineering practice.

3.4.2 Suitability of the code

CODE_BRIGHT is a tool designed to handle coupled THM problems in geological media. The code is able to solve non-saturated multiphase flow under non-isothermal conditions. The equations that govern the THM problem are categorized into four main groups, namely, balance equations, constitutive equations, equilibrium restrictions and definition constraints. Equations for mass balance were established following the compositional approach (Olivella et al. 1994). That is, mass balance is performed for water, air and mineral species instead of using solid, liquid and gas phases. Equation for balance of energy is established for the medium as a whole. The equation of momentum balance for the porous medium is reduced to that of stress equilibrium (Olivella et al. 1996).

The constitutive equations establish the link between the independent variables (or unknowns) and the dependent variables. There are several categories of dependent variables depending on the complexity with which they are related to the unknowns. Basic constitutive laws are divided in thermal, hydraulic and mechanical. The governing equations are finally written in terms of the unknowns when the constitutive equations are substituted into the balance equations. The unknowns are obtained by solving the system of PDE's (Partial Differential Equations) numerically in a coupled way. From state variables, dependent variables are calculated using the constitutive equations or the equilibrium restrictions.

For the numerical treatment of the different terms of the balance equations, the first step is the approximation of the material derivate with respect to the solid as a eulerian derivate, owing to the assumption of small strain rate. Details related to the discretisation of the problem and the numerical technique used can be found in CODE_BRIGHT User's Guide (2009). In summary, it can be mentioned that the numerical approach can be viewed as divided into two parts: spatial and temporal discretisation.

Regarding the boundary conditions of the mechanical problem, forces and displacement rate can be enforced in any spatial direction and at any node. In the hydraulic problem, mass flow rate of water and dry gas can be prescribed at any node, and liquid/gas pressure can be also enforced at any node. Finally, regarding the thermal problem, heat flow and temperature can be prescribed at any node of the mesh (CODE_BRIGHT User's Guide 2009).

For modelling the mechanics of buffer and backfill material, which consist of expansive bentonite clay, a thermo-elastoplastic law, based on BBM (Alonso et al. 1990) which was developed to describe the hydro-mechanical behaviour of partially saturated soils, is used. In the safety assessment SR-Can

(SKB 2006b), the relevance of the thermo-elastoplastic model for highly expansive clays was identified as a subject for developments. The modifications made on this constitutive law, as described in Åkesson et al. (2010a, Appendix C and Appendix D), are results of the investigations made on this topic.

The parameter setting is discussed in detail in the SR-Site THM Data Report (Åkesson et al. 2010b).

3.4.3 Usage of the code

The documentation of CODE_BRIGHT is provided by CODE_BRIGHT User's Guide (2009). The documentation contains a description of the code and the models that are implemented.

CODE_BRIGHT uses GiD system for preprocessing and post-processing. GiD is an interactive graphical user interface that is used for the definition, preparation and visualisation of all the data related to numerical simulations. This data includes the definition of the geometry, materials, conditions, solution information and other parameters. The program can also generate the finite element mesh and write the information for a numerical simulation in its adequate format for CODE_BRIGHT. It is possible to run the numerical simulation directly from the GiD system and to visualise the results without transfer of files. Detailed information will be found in CODE_BRIGHT User's Guide (2009, Chapters CODE_BRIGHT Preprocess and Postprocess).

3.4.4 Development process and verification

CODE_BRIGHT was developed at the UPC in the beginning of the 1990s (Olivella et al. 1994, 1996, Olivella 1995). The code has been verified and validated through comparisons with analytical solutions for a number of problems, see (Olivella 1995, CODE_BRIGHT v3 Verification document 2009). In CODE_BRIGHT v3 Validation document (2009) numerous references are given where CODE_BRIGHT has been used.

The implemented modifications of the BBM-based mechanical constitutive law in the code are only active when mechanical problems are solved using this specific mechanical law. The code modification is contained within the part of the code describing the constitutive law. Thus, the foundation of the code has not been altered by the implementation of the modification. The implementations have been tested and validated for special cases where the solution is known. Where isotropic problems have been solved, the CODE_BRIGHT solutions have been compared to solutions obtained by MathCad implementations. The modifications of the swelling modulus κ_s and critical state line slope parameter M are described in Åkesson et al. (2010a, Appendix C and Appendix D, respectively).

3.4.5 Handling of input data, computational results and scripts

The results from the CODE_BRIGHT models used for THM analyses by Åkesson et al. (2010a) were documented and evaluated within that study. They were used to analyse the saturation time, the homogenisation process and maximum temperatures for different system components. All input files to the CODE_BRIGHT models are stored at Clay Technology's data server (Administrativa dokument\Projekt\THM SR-Site modellering\data\), (Administrativa\Projekt\SKB\SKB SR_SITE\ SR-Site SSM-frågor\data\modeller) and archived at SKB (SKBdoc 1265606 and SKBdoc 1930115, see Table 1-2).

In the data archive the different tasks sorted in specific folders. These folders are divided in two folders, one for all CODE_BRIGHT models and one for all additional documentation (\Task n (description)\ FE-models, \Task n (description)\Other documents).

3.4.6 Rationales for using the code in the assessment

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

3.5 ConnectFlow

3.5.1 Introduction

ConnectFlow is the suite ofWood's (formerly Serco's) groundwater modelling software (Wood 2008a) that includes the NAMMU (Wood 2008b) continuous porous medium (CPM) module and the NAPSAC (Wood 2008c) discrete fracture network (DFN) module. ConnectFlow is also the name given to the concept of nesting CPM and DFN sub-models into a combined CPM/DFN model. A further module, GeoVisage, is a dedicated 3D visualisation application for interpreting the results from ConnectFlow. Hence, ConnectFlow is a very flexible tool for modelling groundwater flow and transport in both fractured and porous media on a variety of scales. NAMMU was originally developed as part of UK Nirex programme. NAPSAC was initially developed as part of the international Stripa project[3,4] (Herbert et al. 1991, Herbert and Lanyon 1992). Integration of the DFN and CPM concepts started as part of UK Nirex programme (Jackson and Watson 1997) and the Äspö Task Force (Holton and Milický 1997). ConnectFlow is now maintained and developed through the international *iCONNECT* club (Holton et al. 2003) (including SKB, Posiva, and Obayashi) and by other commercial users. . It is also noted that ConnectFlow and the geochemical simulation tool PhreeqC have been coupled (Joyce et al. 2015b) thus enabling hydrogeochemical simulations involving chemical reactions. This feature of the model was used in Joyce et al. (2015a) where an extended temperate period was simulated as part of a formal reply to questions posed in the review of SR-Site.

ConnectFlow has a long track-record of being used in the SKB programme since SR 97 (Boghammar et al. 1997, Hartley et al. 1998). Bespoke developments have been made to suit the needs of site modelling and safety assessment calculations (Marsic et al. 2001, 2002). The role of the software in the safety assessment was proposed in SKB (2003) and illustrated in the SR-Can interim assessment (Hartley et al. 2004, SKB 2004). The current use of ConnectFlow is a natural progression from its application in the site-descriptive modelling (Follin 2008). Connectflow version 9.6 is used in the current application.

The simulations have been run on a Linux cluster at Wood (formerly Serco), Harwell, UK. Due to the relatively large user base, the software is of category 3 within the PSAR project.

3.5.2 Suitability of the code

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

3.5.3 Usage of the code

The capabilities of ConnectFlow are described in the Technical Summary Document (Wood 2008a). Input data is supplied to the code as text files and results are output as binary files and as an ASCII log-file which can be checked for errors, warnings and issues such as convergence. The syntax of the input data and the input language is documented in the HTML Command Reference Manual. The code can also be run using a Graphical User Interface (GUI) which is documented by an on-line User Manual. Checking of input files is recorded by the originator and then cross-checked by a second user.

[3] **Herbert A, Gale J, Lanyon G, MacLeod R, 1991.** Modelling for the Stripa site characterization and validation drift inflow: Prediction of flow through fractured rock. SKB Stripa Project Technical Report 91-35, Svensk Kärnbränslehantering AB (Internal document).

[4] **Herbert A W, Lanyon G W, 1992.** Modelling tracer transport in fractured rock at Stripa. Stripa Project Technical Report 92-01, Svensk Kärnbränslehantering AB (Internal document).

3.5.4 Development process and verification

ConnectFlow is maintained and developed under an appropriate QA programme (Wood 2008d). The QA Programme conforms to the international standard BS EN ISO 9001 (2000) and to the TickIT Guidelines. The Concurrent Versions System (CVS) version management system is used to store all source code and test data for ConnectFlow. This automatically logs the author and date of each change to the system, and enables previous versions of the code to be accessed and recreated if necessary. All changes are thoroughly tested, and must be approved by the Software Manager before they are accepted. Through the ConnectFlow QA programme, Wood seeks to continually improve the quality and reliability of the program.

NAMMU has been verified within several international project including HYDROCOIN and INTRACOIN (SKI 1984, 1986, NEA/SKI 1988). NAPSAC has been verified within the STRIPA project (Herbert et al. 1991, Herbert and Lanyon 1992). A full description of the verification of NAMMU and NAPSAC are given in Wood (2008d, e). Testing of combined models is reported in the ConnectFlow Verification Manual (Wood 2008f). Each release of ConnectFlow is verified by running a full test set for all modules of the software with over 200 test cases.

3.5.5 Handling of input data, computational results and scripts

ConnectFlow runs are carried out using data sets written in ConnectFlow's command language. The input files for each run are specified in the header of the data set. Each input file is stored under the project directory on Wood's (formerly Serco's) Linux cluster at Harwell, UK and is either generated by a previous ConnectFlow run or is downloaded from SKB's Trac system (svn/SR-SiteDataStorage). Some input files are processed by Java programs to produce input suitable for ConnectFlow, e.g. the IFZ files for the hydraulic conductor domains (HCD) and the grids for the repository layout. All Java programs and Perl scripts are kept under the project directory on Wood's (formerly Serco's) Linux cluster at Harwell, UK.

Output files are also stored under the project directory on Wood's (formerly Serco's) Linux cluster at Harwell, UK. Some of these are processed by Perl scripts to produce output suitable for delivery to other teams. The final output for delivery is uploaded to SKB's Trac system (svn/SR-SiteDataStorage).

The ConnectFlow input and output data used in the PSAR and SR-Site are archived at SKB (SKBdoc 1256019, see Table 1-2).

3.5.6 Rationales for using the code in the PSAR

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

3.6 DarcyTools

3.6.1 Introduction

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

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

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

DarcyTools is developed through collaborative effort by SKB, CFE AB (Computer-aided Fluid Engineering AB) and MFRDC (Michel Ferry Research&Development Consulting) with SKB as the owner of the code. DarcyTools builds upon earlier development of groundwater models, carried out by CFE AB during the last twenty years. One such early development is represented by Svensson (1991), where predictions of inflows to the Äspö HRL, prior to its construction, are reported. At this time the general purpose equation solver PHOENICS (Spalding 1981) was used. DarcyTools is based on the solver MIGAL (Ferry 2002) and the development work on DarcyTools was initiated early 2001. The first well documented version of DarcyTools is v2.1, which was released in 2004. Version 3.4 is the version used in PSAR. 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 SR-Site (and hence PSAR) version of the code is described in a set of three reports (Svensson et al. 2010, Svensson 2010, Svensson and Ferry 2010).

3.6.2 Suitability of the code

Due to the collaborative (SKB and CFE AB/MFRDC) development of DarcyTools, it was from start decided that DarcyTools should be "the tailor-made SKB code". It is hence not surprising that the key features of the code match the requested capabilities in for example site investigation or glaciation studies. It is beyond the scope of the present text to describe these features (see Svensson et al. 2010) but one may mention: DFN-generation, free surface algorithm, multirate diffusion model and coupled groundwater flow and salt transport. In addition to useful features, a code needs to be efficient. The earlier mentioned unstructured grid in combination with the equation solver MIGAL (an unstructured multigrid solver) ensures that DarcyTools v3.4 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 needs 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, Vidstrand et al. 2010a, b) provide other valuable sources of information.

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

An important part in the usage of the code is the monitoring of the simulation on the computer screen. Convergence parameters, development of variables in control points or profiles are plotted on the screen during the simulation. In v3.4 it is also possible to plot the distribution of variables in specified planes.

3.6.4 Development process and verification

One of the three documents mentioned above (Svensson 2010), deals with verification, validation and demonstration. About thirty simple test cases, most with an analytical solution, are used to ensure that the equations are solved correctly. When a new major version of the code is released, all test cases are updated and checked to ensure both consistency with the old version and to make sure that the new version is correct. Validation is considered to be the process by which the code is shown to agree with measured data ("the right equations are solved"). A number of comparisons with field data are included in the above mentioned report. So far, no attempt to show that DarcyTools conforms to any international QA standard has been made.

3.6.5 Handling of input data, computational results and scripts

Input files are downloaded from svn/SR-SiteDataStorage and stored on the working directory. In this directory, which is backed-up regularly, also output files and scripts for running various parts of the code are stored. DarcyTools results used by other models and analyses within SR-Site are stored in svn/SR-SiteDataStorage.

The DarcyTools input and output data used in SR-Site, and hence PSAR, are archived at SKB (SKBdoc 1256019, see Table 1-2).

3.6.6 Rationales for using the code in the PSAR

DarcyTools 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

The PSAR post-closure safety assessment is based on the same set of Ecolego calculations that supported the safety assessment SR-Site. Ecolego is a flexible software tool for modelling of dynamic systems and performing deterministic or probabilistic simulations. In SR-Site, Ecolego was used for probabilistic and supporting simulations for generating Landscape Dose Factors (LDF's) (Avila et al. 2010). Thus, Ecolego was used as a complement to Pandora (see Section 3.15).

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 being used by companies and institutions all over the world. The version used within the SR-Site project was Ecolego 4.0.

Since Ecolego is a commercial code with a large user-base it belongs to category 3.

3.7.2 Suitability of the code

Ecolego has been designed to maximize 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 mathemathical model is described in detail in Andersson (2010).

3.7.3 Usage of the code

Ecolego has a thorough web-based user guide (www.ecolego.se) which is continuously updated using the Wiki-concept. 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 eventual bugs and request improvements.

The correct usage of the code is assured since Ecolego was used, in the SR-Site project, in close collaboration with the developer of the code (see Avila et al. (2010) for a description of the version used in SR-Site).

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 SR-Site models have been implemented in both Pandora (Simulink, see Section 3.15) and Ecolego to validate the simulation results. The Ecolego software is continuously tested using standard unit testing algorithms.

3.7.5 Handling of input data, computational 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-Site has been stored as an assessment at SKB's subversion server.

Input data used for simulations are stored within the assessment file and originally extracted from the version handled Pandas assessments files representing the base cases at SKB subversion server using Java-scripts. The scripts used to perform batch simulations are archived at Facilia's internal concurrent versioning system (CVS).

The Ecolego input and output data are archived at SKB (SKBdoc 1927863, see Table 1-2).

3.7.6 Rationales for using Ecolego in the PSAR

Ecolego is used since the code is suitable for risk assessments of complex dynamic systems evolving over time with any 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 involve large number of parameters and complex relationships between the inputs and the outputs. In addition, Ecolego enables quick modifications and simulation of large number of assessments.

3.8 ERICA Tool

3.8.1 Introduction

The ERICA Tool was used in SR-Site to estimate dose rates to non-human biota (Torudd 2010). This tool facilitates the use of the ERICA Integrated Approach that can be applied in planned and existing exposure situations (Beresford et al. 2007). The review of the SR-Site assessment by SSM resulted in requests for further information regarding the biota dose rate assessment. To address these requests a supplementary report was produced (Jaeschke et al. 2013). The report is an extension and development of the SR-Site assessment (reported in Torudd 2010) and aimed to address regulator questions. It used an updated, November 2012, version of the ERICA tool. The ERICA Tool is freely available (www.erica-tool.com) and has a large international user base. Since it not written exclusively for the SKB safety assessment, the code is regarded as a category 3 code.

3.8.2 Suitability of the code

The ERICA Tool is a software programme that guides the user through the environmental impact assessment process, keeps records and performs the necessary calculations to estimate dose rates to selected biota. The implementation of the code in SR-Site is described by Torudd (2010) and Jaeschke et al. (2013).

The Tool interacts with a number of databases and other functions that help the assessor to estimate environmental media activity concentrations, activity concentrations in biota, and dose rates to biota. The databases consider the majority of the radionuclides included in Publication 38 of the International Commission on Radiological Protection (ICRP) (ICRP 1983). The ERICA Tool also interfaces with the FREDERICA radiation effects database (www.frederica-online.org), which is a compilation of the scientific literature on radiation effect experiments and field studies, organised around different wildlife groups and, for most data, broadly categorized according to four effect umbrella endpoints: morbidity, mortality, reproduction, and mutation.

The databases of the ERICA Tool are built up around a number of reference organisms. Each reference organism has its own specified geometry and is representative of either terrestrial, freshwater or marine ecosystems. The approach is compatible with that used by ICRP; some of the geometries proposed for the ICRP 'reference animals and plants' are used as defaults in the ERICA Tool.

Some minor updates of the ERICA tools are described in Jaeschke et al. (2013).

3.8.3 Usage of the code

A thorough web-based user guide, found at www.erica-tool.com, is continuously updated. The user guide provides sufficient guidance for the use of the code, with step by step tutorials and also full description of all implemented methods and features. The detailed help assists the user in making appropriate choices and inputs, as well as interpret the outputs. At the same web site, there is also access to other resources such as a forum for support, ideas and answers as well as an issue tracker to report eventual bugs and request improvements.

3.8.4 Development process and verification

The ERICA tool was developed within the ERICA EURATOM project in the area of radiological environmental protection (www.erica-tool.com), by a large consortium of European organisations lead by the Swedish Radiation Safety Authority. Currently the ERICA Tool is being maintained by a consortium comprising the Norwegian Radiation Protection Authority, Environment Agency (England and Wales), Centre for Ecology & Hydrology (UK), IRSN (France) the Swedish Radiation Safety Authority and CIEMAT (Spain). The ERICA Tool is freely available (www.erica-tool.com) and has a large international user base. ERICA is a widely used tool, which is becoming an internationally standardized tool for assessment of doses to non-human biota.

The quantification of uncertainties in the dose estimations with ERICA has played an important role from the very beginning of the tool development; see for example Avila et al. (2004). The accuracy of the dose calculation methodologies implemented in ERICA, as well as the tool itself, have been verified in several studies where predictions using ERICA have been compared with measured data (Beresford et al. 2005, Wood et al. 2008). The ERICA Tool has also participated in several model comparisons exercises (Beresford et al. 2008a, b, 2009, 2010, Vives i Battle at al. 2011) within the IAEA's EMRAS I and EMRAS II programmes. The Bioprota Project (www.Bioprota.org) has investigated the applicability of the ERICA Tool in the context of safety assessment of radioactive waste repositories. In particular, a sensitivity analysis and a knowledge quality assessment of the application of ERICA and similar tools to the assessment of impacts from waste repositories (Smith et al. 2010) was carried out within this project.

In order to assure that there is no difference between the results obtained using the ERICA tool released at 2009 (used in the assessment reported in Torudd (2010)) and the updated version (November 2012), the results in Torudd (2010) and Jaeschke et al. (2013) were compared (Jaeschke et al. 2013).

3.8.5 Handling of input data, computational results and scripts

After a simulation, an ERICA model is saved together with its input data and the results as an assessment file. The updated assessment is reported in Jaesche et al. (2013). Each simulation performed has been stored and is found in SKBdoc 1927863 (see Table 1-2).

3.8.6 Rationales for using the code in the PSAR

The ERICA Tool is used since it is a well-documented and internationally used and reviewed tool for estimation of dose rates to non-human biota.

3.9 FARF31

3.9.1 Introduction

FARF31 (Lindgren et al. 2002) is a code used for radionuclide migration calculations in the far-field, i.e. the geosphere. It is based on a model with a one-dimensional advection-dispersion equation along a, possibly curved, stream tube coupled to a pure diffusion equation in the direction perpendicular to the centroid of the stream tube, for a number of radionuclides. Chain decay and ingrowth are included in the model. The concept of a stream tube can be compared to the combined effect of a large number of individual fractures all sharing the same inlet and outlet. The transversal dimension of the stream tube, the penetration depth, must be chosen by the user.

FARF31 has been used by SKB in the SR 95 (SKB 1996), the SR 97 (SKB 1999) the SR-Can Interim (SKB 2004), SR-Can (SKB 2006b) and SR-Site (SKB 2011) safety assessments of a final repository of the KBS-3 type. In addition, the code has been used by Andra (Andra 2005) and the European Commission's Joint Research Centre (Prváková 2005).

The code was initially developed by SKB in the early 1990's as a submodel of the SKB safety assessment framework Proper. This framework is a collection of codes used for migration and consequence calculations through the near-field, the far-field and the biosphere, and uses standardised methods to transfer data and results between the different submodels. FARF31 has been continuously developed by SKB and subcontractors from its conception until the present version 1.2.1. FARF31 is a Fortran 77 code. In PSAR, a stand-alone version of the code, called from MATLAB scripts, is used.

Since the code has been developed by SKB, the code is belonging to category 4b.

3.9.2 Suitability of the code

The governing equations are solved in the Laplace domain using the groundwater travel time in the longitudinal direction as the independent variable to obtain a unit response function, which is subsequently convoluted with the input function to obtain the output function. A detailed description of the solution method can be found in Norman and Kjellbert (1990).

The FARF31 code has been developed by SKB to be a reasonably accurate, simplified model of the fully three-dimensional far-field transport problem, which still is fast enough to allow for probabilistic calculations. The solution method, based on Laplace transformation of the governing equations and numerical inversion, limits its applicability to cases with constant transport properties, but this poses no problem at the present level of knowledge. However, a different solution method must be used to include colloid facilitated transport in the model. This is possible to handle in a version of the code called FARF33, where the governing equations are discretised in space using a first order finite volume scheme in both the longitudinal and the transversal direction (Vahlund and Hermansson 2006b). In SR-Site, the MARFA code was used for colloid facilitated transport (see Section 3.10). However, in PSAR these calculations are not revisited.

In a dedicated test batch (Appendix B in the FARF31 User's Guide (Lindgren et al. 2002)) and in previous assessments, the capability of solving problems for the expected input data ranges has been shown.

3.9.3 Usage of the code

In the FARF31 User's Guide (Lindgren et al. 2002) the program and its implementation and usage details are explained. Text files are used to pass input data to the code and results from the code. During each run log files are produced, which makes it possible to ensure the right parameter values have been used after the simulation has finished.

3.9.4 Development process and verification

In the validity document (Elert et al. 2004) it is shown that the results are equal to analytical solutions and results from other numerical codes.

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

3.9.5 Handling of input data, computational results and scripts

In PSAR, FARF31 runs are handled with MATLAB scripts. The release from the near-field calculated with COMP23, see Section 3.13, is transferred to FARF31 in the MATLAB scripts. Results from the hydrogeological calculations performed in SR-Site (SKB 2011) with ConnectFlow given as ASCII-files (ptb-files) (SKBdoc 1256019, see Table 1-2) are simply converted to MATLAB input-data.

Input data, results and scripts are stored in Subversion. The used input data and scripts are documented in SKBdoc 1929341 (Table 1-2). The main results are available in SKBdoc 1929341 (Table 1-2).

3.9.6 Rationales for using the code in PSAR

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

3.10 GRISLI

3.10.1 Introduction

GRISLI (GRenoble Ice Shelf and Land Ice model) is a 3D thermo-mechanical ice sheet model with the added capability to also simulate ice streams and ice shelves.

In PSAR, GRISLI is used to reconstruct the maximum extent of the Fennoscandian ice sheet during the Late Saalian glacial maximum (about 140 000 years ago), which is the largest known glaciation in Eurasia of the last 2 million years according to geological records. Several sensitivity simulations were carried out with GRISLI to analyse the effects of e.g. internal model parameters, model resolution and upper boundary condition (i.e. the climate) on the Fennoscandian ice-sheet thickness during the Late Saalian glacial maximum. These simulations constitute the basis for the assessment of the maximum ice sheet thickness, and resulting maximum glacially-induced isostaic pressure, that could exist in the Forsmark region within the time frame covered by the PSAR safety assessment. The model setup, experimental design and results from this study are documented in Colleoni et al. (2014) and Quiquet et al. (2016).

The GRISLI code, written in Fortran, was originally developed by Dr. Cathrine Ritz at Université Grenoble Alpes, Grenoble, France, to simulate the Antarctic ice sheet (e.g. Ritz 1992, Ritz et al. 1997, 2001, Rommelaere and Ritz 1996), but has later also been frequently used for other applications, e.g. reconstructions of Fennoscandian ice sheets (e.g. Peyaud 2006, Peyaud et al. 2007, Alvarez-Solas et al. 2013, Quiquet et al. 2013, Colleoni et al. 2016). In PSAR, the version of GRISLI as of June 2013/ Sept 2014 was used. The code is classified as a category 4b code.

3.10.2 Suitability of the code

The governing equations of ice motion in GRISLI are based on conservation mass, momentum and energy. In GRISLI, three different regions of ice flow are considered: ice sheets, ice streams and ice shelves. Areas of ice sheet (inland ice) are subject to the Shallow Ice Approximation (SIA, Hutter 1983), whereas ice streams and ice shelves are simulated using the Shallow Shelf Approximation (SSA, MacAyeal 1989). In reality, ice streams are glaciological features with widths of a few kilometers,

much smaller than the GRISLI grid size (20 to 100 km). Therefore, the effect of ice streams in GRISLI is parameterized by applying the SSA to areas that have the large-scale characteristics of ice streams, i.e. narrow valleys, thick basal sediment layers saturated by meltwater, and areas with low effective basal pressure.

The inclusion of ice streams and ice shelves is important as these may significantly influence the flow pattern of the ice sheet, and thereby also have a potentially large influence on the resulting ice-sheet thicknesses.

In GRISLI, basal sliding might occur in areas where the base of inland ice is at the pressure melting point. For ice stream regions, basal drag is determined by a friction law, and for ice shelves it is set tonet sum of ice accumulation and ablation, where the accumulation is equal to precipitation and the ablation is parameterized using a temperature-index method. In reality, the ablation of an ice sheet is primarily determined by the surface energy balance. However, because the meteorological qunatities required for calculating the surface energy balance (e.g. net radiation and turbulent fluxes in the lower atmosphere) are usually not known for past climates, it is a feasible approximation to estimate ablation using the surface air temperature. GRISLI also modulates the local climate on the ice-sheet surface during runtime by emplying elevation-dependent changes to the precipitation and temperature.

The spatial distribution of surface air temperature and precipitation used in the GRISLI Late Saalian experiments were obtained from the fully-coupled global simulations using the CESM climate model.

3.10.3 Usage of the code

In the PSAR ice sheet simulations, GRISLI uses three initial conditions, namely surface topography, ice thickness and bed topography, i.e. topography below the existing ice sheets. The model's boundary conditions are geothermal heat flux, global sea-level and climate forcing. The boundary conditions are constant-in-time which results in that the simulated ice sheets evolve toward a steady-state. The model is integrated long enough to ensure that steady-state is reached (typically around 300 ka) on a 20 km horizontal grid covering the Eurasian continent. The output data calculated for each grid point are, e.g.: ice thickness, englacial and basal ice temperatures, ice velocity, sliding velocity, isostatic depression of crust and amount of basal melting.

Description of the first version of the code is provided in Ritz et al. (2001), whereas the model settings and input/output data for the version used in PSAR are documented in Colleoni et al. (2014) and Quiquet et al. (2016).

3.10.4 Development process and verification

The GRISLI code is still under active development. Recently, version 2.0 of the model was released (Quiquet et al. 2018). Compared to the model version used in PSAR, the current version includes an explicit flux computation in the transition zone between grounded and floating ice, but is otherwise very similar.

Both the first and second versions of the code have been validated against the present-day geometry of the Antarctic ice sheet (Ritz et al. 2001, Quiquet et al. 2018). Both studies show that the simulated present-day distributions of grounded and floating ice on Antarctica agree reasonably well with observations. GRISLI has also participated in several model intercomparison projects (Calov et al. 2010, Edwards et al. 2014, Koenig et al. 2015, Nowicki et al. 2016, Goelzer et al. 2019). In the most recent interpomparison project (ISMIP6, Nowicki et al. 2016), the projected sea-level rise by the end of the century in GRISLI comply well with other ice-sheet models, even more complex ones (Edwards et al. 2014, Goelzer et al. 2019).

3.10.5 Handling of input data, computational results and scripts

Both input and output data are dealt with in NetCDF (Network Common Data Form) and ASCII format. To date, there are many applications available for the processing and visualization NetCDF data, e.g. Climate Data Operators (CDO), NetCDF Operators (NCO), Ncview, Grid Analysis and Display System (GrADS), Python and MATLAB. Data are archived in SKBdoc 1927730 (see Table 1-2).

3.10.6 Rationales for using the code in the PSAR

The GRISLI code was selected for the PSAR safety assessment for the following two reasons:

1. The model has previously been used to reconstruct the extent of the Fennoscandian ice sheet during the Late Saalian glacial maximum (e.g. Peyaud 2006). Most other ice sheet models have not yet been used to simulate this time period. From the previous simulations of the Late Saalian ice sheet, a very large amount of work regarding setting up the model for this time period, was already available at the start of the analysis performed for the PSAR assessment.
2. The adaptation of the SIA approximation for computing the ice velocities over most parts of the ice sheet implies that the model is computationally cheap, and so allows for a large number of sensitivity simulations to be carried out. The large number of sensitivity simulations were crucial for the PSAR assessment of maximum possible ice-sheet thickness at Forsmark during future glaciations.

3.11 MARFA

3.11.1 Introduction

In SR-Site, MARFA 3.2.2 (Painter and Mancillas 2009) which is a Fortran 95 code for radionuclide migration calculations in the geosphere, was used. It represents transport along one-dimensional flow-paths extracted from a ConnectFlow or similar flow model. The solution method is a particle-based Monte Carlo approach (Painter et al. 2008). Advection, longitudinal dispersion, limited or unlimited diffusion in rock matrix adjacent to the flow path, equilibrium sorption, and decay/ingrowth are represented. Colloid-facilitated transport may be represented in MARFA by appropriate manipulation of input parameters. Full heterogeneity is supported. That is, the code allows an arbitrary (user input) number of flowpaths and each flowpath may be divided into an arbitrary number of segments with different flow and transport properties within each segment. Different segments may have different retention models (e.g. matrix diffusion in some segments and equilibrium sorption in others). MARFA 3.2.2 also supports temporal variability in flowpath properties. Specifically, different flow velocities and non-flow related transport parameters may be entered for different time periods. However, the three-dimensional flowpath trajectories themselves are assumed fixed in MARFA 3.2.2.

MARFA is a category 4b code.

3.11.2 Suitability of the code

MARFA 3.2.2 accurately represents processes that are expected to be dominant transport processes in the Forsmark geosphere, similar to the FARF31 code (Section 3.9). MARFA was developed to represent certain features, events and processes that are not represented in the FARF31 code. Specifically, the solution method in MARFA does not require the flowpath to be homogenised into an effective constant-property pathway. Theoretical justification for such homogenisation has been demonstrated for single nuclides, but not for radionuclides linked through decay chains. In addition, MARFA also allows for different retention models in different parts of the flowpath, thus making it possible to represent sorption in backfilled tunnels or near-surface soils. MARFA also allows flow velocities and retention parameters to change with time.

3.11.3 Usage of the code

Data input to MARFA is through a series of input files, as described in the MARFA User's Manual (Painter and Mancillas 2009).

3.11.4 Development process and verification

MARFA was developed at the Geosciences and Engineering Division (GED) of Southwest Research Institute (SwRI) in Texas, USA. The GED conducts all quality affecting activities in compliance with applicable requirements of Title 10 of the US Code of Federal Regulations Part 50, Appendix B (10 CFR Part 50, Appendix B; Domestic Licensing of Production and Utilization Facilities, Quality

Assurance Requirements for Nuclear Power Plants and Fuel Reprocessing Plants). More specifically, quality affecting research and development activities related to geological disposal of high-level radioactive waste and spent nuclear fuel comply with the requirements of 10 CFR Part 63, Subpart G (Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada, Quality Assurance). The industry implementing standard for 10 CFR Part 50, Appendix B is American Society of Mechanical Engineers (ASME) NQA-1, Quality Assurance Requirements for Nuclear Facilities Applications (1986).

Software is developed, controlled, and modified using GED Technical Operating Procedure (TOP)-018, Development and Control of Scientific and Engineering Software. This procedure invokes the US Nuclear Regulatory Commission (NRC) regulatory guidance documents NUREG/BR-0167, Software Quality Assurance Programs and Guidelines, and NUREG-0856, Final Technical Position on Documentation of Computer Codes for High-Level Waste Management. Furthermore, TOP-018 identifies appropriate processes and documentation to control appropriate elements of the software development process. These measures include but are not limited to preparation of a software requirements description, software development plan, software validation plan, software release notices, software change notices, and similar documentation, as appropriate taking into consideration the size, complexity, and importance of the software being developed or modified. TOP-018 also provides guidance on preparation of a user guide.

After SR-Site, hosting of MARFA has been changed, and hence also the development process.

MARFA is currently developed and maintained by Amphos 21 in Barcelona, Spain using a test-driven development cycle. After each set of code modifications, a release candidate is prepared and the development will enter a testing phase. Regression tests are implemented to ensure new code changes do not alter functionality from previously existing code. New validation tests will be added when new functionality is developed or when bugs are found in uncovered portions of code. After all regression tests have been passed by a release candidate, the new software is released on the software repository and versioned according to the versioning system. Software enhancement tasks such as code refactoring, memory footprint reduction, etc. are included under maintenance tasks.

Trello, a web-based project management application, is used to develop a new feature and for bug tracking. Before a new functionality is added to existing software, a request to add new capability must be solicited and added as a task on Trello. A software change request includes integrated sub-tasks of development, refactoring, testing, release and update of the user manual. Trello boards are used to provide issue tracking and to request a new feature. Issue tracking will follow the agile development paradigm (creating issues of issue type “Bug”). A task labeled as bug will be added on Trello. A bug fix is followed by the subsequent tasks of refactoring, testing, release and update of the user manual.

The default code repository is hosted on Bitbucket cloud, which is a web-based hosting service. The development repository is private with limited pull privileges granted to authorised MARFA users. The release repository is public and open. Version control is maintained through Mercurial, which is a freely distributed integrated source control management tool. The development is usually carried out by creating a development branch on which the new feature can be developed, tested and after being verified merged to the main repository branch.

Software validation tests are summarized in the MARFA user’s manual (Painter and Mancillas 2009), which is included in a open Bitbucke repository.

3.11.5 Handling of input data, computational results and scripts

MARFA requires flowpath definitions, radionuclide mass release rates from the near field, and retention parameters for the far field. MARFA is designed to directly accept ConnectFlow (see Section 3.5) ptv-files to define flowpaths. However, some modelling cases required the ConnectFlow-generated ptv-files to be modified to remove certain segments of the calculated flowpaths or to remap rock type numbering. Non-flow related transport parameters are input through the definition of certain parameters of the retention model. These are input through an ASCII file as described in the MARFA users manual (Painter and Mancillas 2009). Non-flow related transport parameters sampled with the @RISK code (add-in to Microsoft Excel) were reformatted in the MARFA input format. Similarly, radionuclide release rates from COMP23, Section 3.13, were reformatted to the required MARFA

input format. MARFA generates results in units of Bq/yr for each radionuclide. These results are saved in ASCII files and were also converted to units of Sv/yr for display purposes using SR-Site landscape dose factors (LDF's) for the temperate period. A complete input/output set for each MARFA calculation completed in support of SR-Site/PSAR is archived in the QA system of the Geosciences and Engineering Division of Southwest Research Institute (for growing pinhole cases) and in SKB's record management system (SKBdoc 1256019, 1266150, see Table 1-2).

3.11.6 Rationales for using the code in the PSAR

The SR-Site/PSAR team has selected MARFA for the SR-Site/PSAR safety assessment since it was specifically designed to integrate with the safety assessment workflow used by SKB. In contrast to FARF31 the MARFA code supports full spatial variability for all pathway properties as well as colloidal-facilitated transport. The results produced by MARFA have been shown to be in good agreement with results from other codes, for example FARF31.

3.12 MATLAB

3.12.1 Introduction

MATLAB (MathWorks 2010a) is an interactive environment and computing language for numeric computation, analysis and visual presentation. MATLAB has been developed since the late 1970's and is globally widespread. MATLAB has been used for a variety of tasks in SR-Site for instance, migration calculations in all parts of the repository system (COMP23, Section 3.13), landscape models (Pandora, Section 3.15) and FPI-calculations (Section 3.14), and also for pre- and post-processing of data and their visualisation.

Simulink (MathWorks 2010b), an extension integrated with MATLAB, is an environment for multidomain simulation and model-based design for dynamic and embedded systems. It provides an interactive graphical interface to MATLAB and implements MATLAB with a customisable set of block libraries.

While MATLAB and Simulink on their own are regarded as a category 3 code, the advanced applications using MATLAB are regarded as category 4 codes.

3.12.2 Suitability of the code

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

3.12.3 Usage of the code

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

3.12.4 Development process and verification

This is a commercial code and the developer grant for the development process and verification of the code. The large number of users worldwide warrants swift reactions on programming errors.

3.12.5 Handling of input data, computational results and scripts

In the assessment, MATLAB is not used as a separate code, instead MATLAB provides mathematical solving capability and, together with Simulink, graphical environment for the codes developed or tuned.

3.12.6 Rationales for using the code in the PSAR

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

3.13 MATLAB – COMP23

3.13.1 Introduction

In the PSAR, an implementation of the COMP23 model written in MATLAB/Simulink, is used for the near-field migration calculations. This implementation of the COMP23 is also called Compulink (Vahlund and Hermansson 2006a).

COMP23 has been used by SKB in the SR 95 (SKB 1996), the SR 97 (Lindgren and Lindström 1999, SKB 1999), the SR-Can Interim (SKB 2004), SR-Can (SKB 2006b) and SR-Site (SKB 2011) safety assessments of a final repository of the KBS-3 type. A closely related code, NUCTRAN/NUCFLOW, (which origins from the same source but allows for multiple sources as opposed to COMP23 which only handles single sources) was used in the safety assessment SAFE of the SFR repository for operational waste (Lindgren et al. 2001). In addition, the code has been used by Andra (Andra 2005) and the European Commission's Joint Research Centre (Prváková 2005) and, to some extent, by the Lithuanian Energy Insitute (LEI) (Neerdael and Finsterle 2010).

COMP23 (Cliffe and Kelly 2006) is originally a Fortran77 code used for radionuclide migration calculations in the near-field (the canister and the engineered systems) and includes models for fuel dissolution, handling of element specific solubility, and migration through advection and dispersion in the different parts of the engineered system. The code was initially developed as NUCTRAN (Romero 1995) and was subsequently incorporated into the SKB safety assessment calculation framework Proper as the submodel COMP23. Proper is a collection of codes used for migration and consequence calculations through the near-field, the far-field and the biosphere and uses standardised methods to transfer data and results between the different submodels. COMP23 has been continuously developed by SKB and subcontractors until the present version 1.2.2.

The code is considered a category 4b code.

3.13.2 Suitability of the code

COMP23 has been developed by SKB with the main objective to solve the problem at hand and includes all essential models needed when modelling radionuclide migration through the engineered system. Some of the models have been used temporarily in the development process of the KBS-3 repository and can be regarded as being obsolete based on the present level of knowledge. The code contains for instance several models of different complexity used to calculate the dissolution rate for the fuel matrix. However, for the PSAR a linear model is used, which corresponds best to the present level of knowledge of the actual processes suggested in the **Data report** and the **Fuel and canister process report**. For the solubility limits inside the canister which is a mechanism limiting the concentration inside the canister, a shared solubility model is used where the solubility limit for an element is shared proportionally between the different isotopes of the same element. For radionuclides embedded in the metal parts of the fuel assemblies the releases are determined by constant corrosion rates. Sorption coefficient, diffusivity and porosity are given for each nuclide which allows cations and anions to be treated differently. The validity of the different models used in the code is discussed in the **Fuel and canister process report** and the **Buffer, backfill and closure process report**.

The spatial discretisation used in the modelling of the KBS-3 system (the sub-division of the near-field into compartments) is described in appendix in the **Radionuclide transport report**. The discretisation is manly based on an earlier study (Lindgren and Widén 1998) where different discretisation techniques have been tested in order to find a discretisation that is coarse enough to allow for the problem to be solved using probabilistic calculations, but yet fine enough allowing for the problem to be solved with acceptable accuracy. In order to be able to have a relative coarse spatial discretisation, analytical expressions are possible to use at the mouth of the canister defect and at the fracture bentonite interface (Neretnieks 1986, Romero 1995, Kelly and Cliffe 2006).

In a dedicated test batch (Lindgren et al. 2008), in the validity document, (Kelly and Cliffe 2006) and in previous assessments, the capability in solving problems for the expected input data ranges has been shown. Compulink uses a subset of the COMP23 test batch (Vahlund and Hermansson 2006a).

3.13.3 Usage of the code

In the COMP23 user's manual (Romero et al. 1999, Cliffe and Kelly 2006) the program and the models implemented are explained in detail. For the MATLAB-version used in the PSAR (Vahlund and Hermansson 2006a) provides additional documentation on the usage. MATLAB scripts are used to handle input and output.

3.13.4 Development process and verification

In a validity document (Kelly and Cliffe 2006), the features of the code are presented and some of these are benchmarked against analytical solutions and in some cases to other codes. In addition to the validity document, a test batch (Lindgren et al. 2008, Vahlund and Hermansson 2006a) has been prepared in which the features of the code are demonstrated both for simple test cases which can be verified with analytical solutions or other codes and also for realistic KBS-3 cases using realistic data. Using the test batch the accuracy between different versions may be verified to ensure that code modifications does not change the capability of the code to solve the problem at hand.

The Matlab/Simulink version of COMP23 uses Subversion for version handling. The Fortran version of the COMP23 uses the version control system SCCS (Boghammar 1999) and batch scripts are used to set up the computational environment.

3.13.5 Handling of input data, computational results and scripts

In this section it is described how data are passed between COMP23 and other models identified in the AMF, see Figure 2-1 and Figure 2-2. Table 3-1 summarises the data and reference to report and section where the passing of data to COMP23 is described and if other model activities are performed to obtain the input data. The used input data and scripts are version controlled in Subversion and documented in SKBdoc 1929341 (Table 1-2). The results are stored in Subversion and the main results are available in SKBdoc 1929341 (Table 1-2).

3.13.6 Rationales for using the code in the PSAR

The PSAR team has selected the MATLAB/Simulink version of COMP23 code for the PSAR safety assessment since it has been designed to solve the radionuclide transport problem at hand and since the knowledge of the code is good.

Table 3-2. Input data passed to COMP23.

Data	Other model activity	Data passing
Inventory for RN transport (DR 3.1)		Subversion, **Data report** Section 3.1
IRF, CRF and Corrosion time for metal parts (DR 3.2)		Subversion, **Data report** Section 3.2
Fuel conversion (DR 3.3)		Subversion, **Data report** Section 3.3
Solubility data (DR 3.4)	Solubilities, Section 3.21	Subversion
Time for large defect (DR 4.3)	Corrosion calculations (incl. buffer erosion), Section 3.3	Subversion, **Data report** Section 4.3, (SKBdoc 1927770)
Geometries		**Underground openings construction report, Canister production report**, **Buffer production report**, **Data report** Section 4.1
Flow related migration parameters (DR 6.7)	Hydro, Section 3.5 (Connectflow)	Subversion (ptb-files), **Data report** Section 6.7 (SKBdoc 1256019)
Density and porosity of buffer and backfill (DR 5.1)		Subversion, **Data report** Section 5.1
Migration data of buffer and backfill		Subversion, **Data report** Section 5.3

3.14 MATLAB – FPI

3.14.1 Introduction

The PSAR post-closure safety assessment is based on the same set of Matlab-FPI calculations that supported the safety assessment SR-Site.The full perimeter intersection criteria (FPI) were used in the safety assessment SR-Can (SKB 2006b) as a proxy for large fractures. This enabled a quantitative estimate of the number of canisters that might fail due to earthquakes.

Using site descriptive models as input, the codes compute the probability of intersection between fractures, idealised as infinitely thin, circular discs, and either canisters, deposition holes or tunnels of various shapes and orientations (Munier 2010). The critical fracture radii, i.e. radii sufficiently large to host slip exceeding the canister failure criterion, are dependent on the distance to deformation zones and the dip of the fracture, as demonstrated in Fälth et al. (2010). Combined with estimates of earthquake frequencies (e.g. Bödvarsson et al. 2006) it is possible to compute an average number of potentially damaged canister for various time frames.

The codes are implemented as MATLAB (MathWorks 2010a) scripts (see also Section 3.12), using the parallel processing toolbox (MathWorks 2010c) for computation speed. A few subroutines were compiled in C++ for additional speed, using the compiler Visual Studio (Microsoft 2008). The version of the code used in SR-Site is “version SR-Site”.

The methodology used to estimate, with simulations, the number of canister positions intersected by critical fractures is presented in Munier (2010). For these simulations, Matlab version R2008b (v. 7.7), was used. However, the simulation times were extremely long and prior to SR-Site, the decision was made to utilize parallel processing for which Matlab R2010b (v. 7.11) resp. Processing toolbox R2010b (v. 5.0) was used. To utilize parallel processing for the calculations in SR-Site only modest modifications of the codes used in Munier (2010) were needed. The codes used in SR-Site are therefore broadly identical to those previously used with the difference that additional script was added to call the parallel calculation and some script to handle the parallel output. All other subroutines were left unchanged.

Matlab-FPI is considered as a category 4b code.

3.14.2 Suitability of the code

The codes were tailor-made for the sole purpose of computing fracture/canister intersection probabilities. The method is described in Munier (2010).

The context has been described in detail in several SKB reports (e.g. La Pointe et al. 1999, Bäckblom and Munier 2002, Munier and Hökmark 2004, SKB 2010d), publications (La Pointe et al. 2002) and conference contributions (e.g. Fälth et al. 2007, 2008, Hökmark et al. 2008, Munier et al. 2008, Munier 2011) and summarized in SKB (2011, Section 10.4.5) and **Geosphere process report**, Section 4.3.4.

Data report, Section 6.3, presents a summary of the assumptions regarding crack geometries, size distributions, spatial distributions, etc. as described by Fox et al. (2007). The various assumptions, basically based on various types of uncertainties (see **Data report**, Section 6.3 for discussion), have led to a broad dropout in the number of critical canister positions. However, SKB chose the cautious principle of consistently applying the values (“parameters”) which were the worst results in terms of long-term safety.

3.14.3 Usage of the code

The codes require MATLAB (see also Section 3.12) and the parallel processing toolbox. The compilation of certain subroutines to C++ was targeted to a 64 bit platform and would need to be recompiled to run on a 32 bit platform. The code is documented in Munier (2010).

3.14.4 Development process and verification

The notion of using full perimeter intersections as proxies for large fractures was originally introduced in Munier (2006) in which the terminology, geometrical framework and first versions of the codes were presented. In Munier (2007), a sensitivity analysis was published together with some fundamental benchmark cases (Hedin 2008). The number of cases to consider, and their output, forced a radical rewriting of the codes and a need to compile some slow routines into native C++. These early reports were complemented in Munier (2010) with a large number of analytical and semi-analytical benchmarks (e.g. Hedin 2011), more sensitivity analyses and an application to both the Forsmark and Laxemar sites. The codes, presented in Munier (2010), were radically rewritten to enable parallel processing, in particular with regards to simulation logic. The versions of the codes in Munier (2010) are those used in SR-Site though the simulation output has been complemented with additional realisations to stabilise results further

Since "Matlab-FPI" was developed for a problem unique to SR-Site, verification against other codes can not be done. One can however evaluate whether the code is accurate, by setting up a number of idealized cases for which there exists analytical solutions. In Munier (2010), the methodology report for FPI simulations, in a dedicated section, a large number of benchmark tests are used to verify that the codes calculate the idealized calculation cases correctly (Munier 2010, Chapter 5). However, going from idealized cases to a model with complete geometries of tunnels and deposition holes, is a relatively large step. In parallel with the development of the FPI codes, SKB therefore developed a semi-analytical solution, (Hedin 2008) against which the FPI codes could be verified.

The calculations of utilization and some idealized calculation cases, however, also posed a challenge and a stereological, semi-analytical solution was therefore implemented to mimic the simulation flow in Matlab-FPI.

3.14.5 Handling of input data, computational results and scripts

There are several sources of input to the simulations. The most important ones are the DFN models for each site. All DFN models of the site description reside in SKB's model database as Microsoft Excel sheets, described in detail in the **Data Report**. However, the FPI codes require ASCII input files with a special formatting. These ASCII-versions of the DFN models are stored together with the MATLAB scripts.

The output also consists of ASCII-files of various formats. These are concatenated into Workbooks in Statistica (Statsoft 2009) in which they are analysed. Statistica also provides the graphical output in terms of tables, diagrams and charts.

All files, which includes compiled subroutines, MATLAB scripts, input, output and Statistica workbooks are handled in Subversion, and are archived at SKB (SKBdoc 1264530, 1264531, 1264532, see Table 1-2).

The entire development of the FPI codes, which includes input (refers to the direct inputs in the form of ASCII versions of DFN models and tunnel geometries), m files, compiled modules, output, as well as benchmarks were quality assured in Subversion (Murphy 2007) using a so called "Shell extension" to Microsoft Windows (Küng and Onken 2009). The codes used in SR-Site constituted a special "branch" in Subversion with number "2690". To further improve traceability, the codes were archived as zip archives in SKBdoc record management system, Table 3-3.

Table 3-3. Archived data, Matlab-FPI.

Archived data	Location	Size
EFPC Development and Benchmarks- Matlab scripts	SKBdoc 1292572	1.38 GB
EFPC modelling in SR-Site – Matlab scripts [Including DFN data listed under "SR-Site Data report"]	SKBdoc 1292573	968 MB
EFPC/FPI modelling – General Matlab codes	SKBdoc 1292574	16 kB

3.14.6 Rationales for using the code in the PSAR

The FPI codes were thoroughly tested within the framework of SR-Can and shown to be adequate for the intended purpose. Models and scripts have been successively developed and backwards traceability is thereby warranted. The assessment team still considers the FPI codes adequate to fulfil the purpose of the simulations and has therefore chosen to continue using the FPI codes as the main tool for analyses of canister/fracture intersection probabilities.

3.15 MATLAB – Pandora

3.15.1 Introduction

The PSAR post-closure safety assessment is based on the same set of MATLAB – Pandora calculations that supported the safety assessment SR-Site.MATLAB-Pandora is a tool for implementation of mathematical models and for performing deterministic and probabilistic simulations with these models. In SR-Site, the software package Pandora was used for deterministic simulations for derivation of the Landscape Dose Factors (LDF's) (Åstrand et al. 2005, Avila et al. 2010, Ekström 2011). Pandora is an extension of the well-known codes MATLAB and Simulink (Mathworks 2010a, b). Pandora simplifies the development of compartment models consisting of large systems of ordinary differential equations and the handling of radionuclide decay chains. The Pandora tool comprises a library of Simulink blocks that facilitates the creation of compartment models, a Manager as an aid in the model building phase and a standalone assessment tool called Pandas for the model simulation phase. Pandora has been developed by Facilia AB and financed by SKB and Posiva OY. Pandas and the Manager have been financed by SKB alone. Pandora is also used for biosphere modelling by Posiva OY. In SR-Site, Pandora svn revision number 5172 was used.

Pandora is considered as a category 4b code.

3.15.2 Suitability of the code

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

- handling of large sets of parameters,
- handling of time evolving parameters,
- representation of discrete transitions between states,
- handling of large number of radionuclides and decay chains,
- consideration of time evolving and spatially distributed discharges,
- version handling of parameters, models and assessments,
- capability to perform probabilistic simulations and sensitivity analysis.

Pandora extends the Simulink graphical user interface as to allow the user to easily inspect and modify the conceptual and mathematical models implemented. The equations on which the model is built are described in Andersson (2010).

3.15.3 Usage of the code

The Pandora code has an internal user guide with step by step tutorials as to build models as well as a general description report (Ekström 2011), which provides sufficient guidance for the additional functionalities that have been incorporated to the commercial codes MATLAB and Simulink. MATLAB and Simulink are well documented and has good support and updating is provided by the developers (Mathworks 2010a, b).

The path to build a landscape model starts by creating a library of ecosystem models in Pandora, which facilitates handling several instances of the ecosystem models in the landscape model. For each landscape object, a Simulink subsystem is created, which includes models of all ecosystem

types that may exist in the object during the whole simulation period. An eventual discrete transition between ecosystem models is implemented using switches available in Simulink. The decay and ingrowth of radionuclides in decay chains are handled with the help of the Pandora Radionuclide block.

For integrating the model, the user can choose from a large list of solvers available in Simulink, including solvers that are appropriate for stiff systems of equations with discrete events. In SR-Site the solver ode15s was used, this due to the high stiffness of the implemented models. The activity concentrations and doses were calculated from the amounts of activity in different compartments predicted with the Pandora model by using a post-processing routine created in MATLAB and incorporated with Pandas assessment. Since Pandora is integrated with the assessment tool Pandas, it also allows for performing sensitivity and uncertainty analyses of the implemented models.

3.15.4 Development process and verification

Pandora has been benchmarked, tested and compared with other similar tools (Åstrand et al. 2005, Ekström 2011). The solutions with the predecessor of Pandora (Tensit) were compared with analytical results, as well as with numerical results obtained with other simulation tools (Jones et al. 2004, 2005). These comparisons have shown that Pandora provides reliable solutions.

3.15.5 Handling of input data, computational results and scripts

In SR-Site, Pandora runs were handled with Matlab scripts. Input data (universal constants, time specific-, site specific- or generic parameter values) were transferred from Excel tables to Pandora in the Matlab scripts.

Input data, results and scripts are stored at SKB's subversion server. These files are archived in the SKB record management system (SKBdoc 1927863, see Table 1-2).

3.15.6 Rationales for using the code in the PSAR

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

3.16 MIKE SHE

3.16.1 Introduction

The PSAR post-closure safety assessment is based on the same set of calculations that supported the safety assessment SR-Site. In SR-Site, MIKE SHE (Système Hydrologique Europeen) was used for hydrology and near surface hydrogeology calculations. MIKE SHE makes it possible to model the integration between surface water, groundwater and evaporation processes and makes it possible to describe and understand the complexity of the water flows in the surface system. The MIKE SHE model provides the dose-model with data on water fluxes in and between different compartments of the dose-model.

MIKE SHE is 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; saturated zone, unsaturated zone, overland flow, evapotranspiration and channel flow, Figure 3-2, in which the water flow is calculated separately. 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.

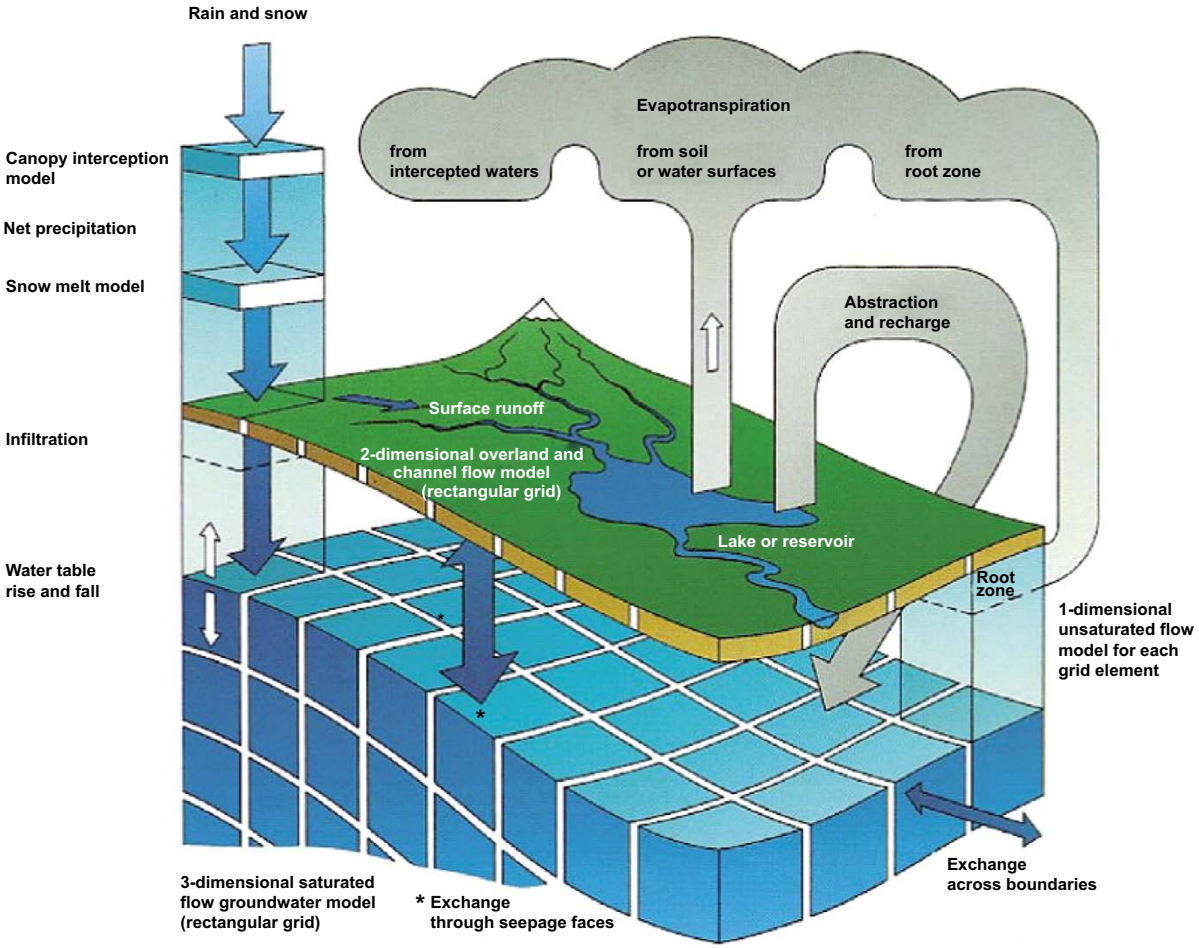

Figure 3-2. *The MIKE SHE model (Abbott et al. 1986).*

MIKE SHE Version 2009 (DHI 2009) was used within the SR-Site modelling. The system is certified for Windows 2000 Professional and Windows XP Professional X64 Edition. MIKE SHE was also used in SR-Can but the code has been developed since then. The coupling between the river flow model and the groundwater flow model in the present version has been updated, so that the water can be transported from the aquifer to the river either via the bottom sediment or over the river bank, as well as allowing water to flood from the river to the ground surface and then infiltrate. Also the evapotranspiration module has been developed. In the MIKE SHE version 2009 it is possible for plants to extract water from the saturated zone which better describes the water turnover in wetlands (Vikström and Gustafsson 2006). It is possible to define a water tolerance for each vegetation type, if the water tolerance is high the plant can extract all its water from the groundwater zone.

MIKE SHE was used in the hydrological and near surface hydrological modelling within SR-Site. The SDM MIKE SHE model (Bosson et al. 2008) has been the basis for the models developed within the framework of SR-Site where both models describing present and future conditions have been developed. Different climate cases and the effect on the hydrology of the shore line displacement and development of the landscape have been analysed. The MIKE SHE modelling is reported in Bosson et al. (2010) and Lindborg (2010).

The code is commercial and is regarded as a category 3 code.

3.16.2 Suitability of the code

MIKE SHE is an advanced integrated hydrological system capable to simulate both surface and groundwater with the same precision as models focused on either groundwater or surface waters. The model is able to simulate the interaction between the surface water and the groundwater which

is important when studying potential flow paths from the repository, i.e the water flow from the geosphere to the biosphere. Groundwater exchange with repository tunnels is possible by a coupling between MIKE SHE and MIKE URBAN (see e.g. Mårtensson and Gustafsson 2010). The coupling can be used both for studies amiing at analyzing the effect of groundwater extraction on the the surface hydrological system and for analyzing the flowpath and flow length of inflowing groundwater to a repository.

The precipitation can either be intercepted by leaves or fall to the ground. The water on the ground surface can infiltrate, evaporate or form overland flow. Once the water has infiltrated the soil, it enters the unsaturated zone. In the unsaturated zone, it can either be extracted by roots, and leave the system as transpiration, or it can percolate down to the saturated zone, see Figure 3-2. MIKE SHE is fully integrated with a channel-flow program, MIKE 11. When using the MIKE 11 code together with MIKE SHE, the two programs run simultaneously allowing for water exchange between the two codes during the whole simulation. The water exchange between M11 and MIKE SHE is further described in Gustafsson et al. (2009).

Based on the calculated flow field, particle tracking calculations (in the saturated zone) and advection-dispersion calculations can be performed. Within the SR-Site application both particle tracking and advection-dispersion calculations have been performed. The solute transport in the advection-dispersion module can be calculated for all the components (river, overland, unsaturated zone, groundwater).

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

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

There is a direct coupling between MIKE SHE and the GIS program ArcMap which is part of the ArcGIS framework. This is a large advantage since most of the input data to the present modelling can be obtained in GIS format. It is possible to use both shape-files and ESRI-grid files as input. Both pre- and post-processing can be made in the ArcGIS program. The program has been developed to calculate the integrated ground- and surface-water system (flow and transport in porous medium, the unsaturated zone and flow and transport of surface water). Hence, the parameter ranges used when simulating are within the ranges for which the program is valid.

3.16.3 Usage of the code

The MIKE SHE user manual (DHI 2009) 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 describes in detail the individual tools and dialogs the user is encountered to when working in 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.

The MIKE SHE user manual follows as a pfd-file with the installation media. The manuals are not available in a printed version. The documents are updated when new releases of the software is available.

3.16.4 Development process and verification

The MIKE SHE model has its origin in the SHE model, Systèm Hydrologique Européen, which became operational 1982. The model was developed by three organisations; the British institute of Hydrology, the French consulting company SOGREAH and the Danish hydraulic institute, DHI. Today DHI markets the MIKE SHE code. The code is developed as new modelling ideas and needs are identified by the users. The latest version of the model is MIKE SHE version 2019.

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

Many organisations have reviewed and evaluated the MIKE SHE code. MIKE SHE has been selected as the best modelling tool for integrated groundwater/surface water modelling in many independent reviews, (e.g. CDM 2001). Each review has had different objectives and has used different criteria in the review process. A number of references are available at DHI website (www.dhigroup.com). Since 2011 when SKB handled in SR-Site several scientific studies where MIKE SHE is used as the main modelling tool has been published (Berglund et al. 2013, Bosson et al. 2012, 2013, Johansson 2015, 2016, Jutebring Sterte et al. 2018, 2021).

3.16.5 Handling of input data, computational results and scripts

Input data is supplied to the code as text files, shape-files or ESRI-grid files. Result files are time series files, *.dfs0 or grid-files, *.dfs2 and *.dfs3. Both dfs0-files, dfs2-files and dfs3-files are easily converted to text files. The dfs2-files can also directly be converted to GIS-format, shape-files or ESRI-grid files. An ASCII log-file is produced for each simulation, this file can be used to check for errors, warnings and issues such as convergence. The MIKE SHE model can also be run using a Graphical User Interface (GUI) which is documented by an on-line user manual.

Several modelling activities have provided the various external input data and models required for the SR Site hydrological and near surface hydrogeological numerical modelling. The MIKE SHE SDM model is the starting point for all model cases simulated within the SR-Site MIKE SHE modelling. The input data used in the SR-Site MIKE SHE modelling is described in Bosson et al. (2010).

All time series data from the site investigations, used as input data to the MIKE SHE model, are stored in the SKB Sicada database. Spatial distributed input data to the MIKE SHE models are stored in the SKB GIS database. Models and data from other scientific disciplines in the SR-Site project that are used in the MIKE SHE SR-Site modelling are stored at SKB's subversion server.

The MIKE SHE model generates numerous result data files. For practical reasons the model result files cannot be uploaded on svn. A separate server at SKB has therefore been in use for storing the MIKE SHE results files (G:\skb\modellering\mikeshe). The scripts used in MIKE SHE for SR-Site are archived at SKB (SKBdoc 1927863 , Table 1-2).

Details about all input data to the MIKE SHE SR-Site model and references to specific data extractions from each database mentioned above are found in Bosson et al. (2010).

3.16.6 Rationales for using the code in the PSAR

MIKE SHE is regarded as a suitable code for solving the problem at hand, since it is a well documented and internationally used and reviewed tool for calculating waterflows in the surface system.

3.17 Numerical GIA model

3.17.1 Introduction

The GIA (Glacial Isostatic Adjustment) code is used to calculate the isostatic adjustment of the solid earth due to loading by ice and water during a glacial cycle. The gravitationally-consistent redistribution of water within the oceans is a central component of the algorithm, allowing accurate relative sea-level and shoreline migration to be calculated.

In PSAR the GIA code is used to reconstruct relative sea-level and shoreline positions in the region of interest. It is also used to carry out sensitivity tests regarding e.g. the influence of earth and ice model parameters on the output, 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 et al. 2002, Bassett et al. 2005), investigating the effect of 3D earth structure on GIA predictions (Whitehouse et al. 2006), and identifying present-day melt sources and constraining the recent mass balance of polar ice sheets (Mitrovica et al. 2001, Tamisiea et al. 2001, 2003). The GIA code was also used for the SR-Can and SR-Site safety assessments (SKB 2006a, SKB 2010c).

The GIA code is a category 4b code, written in Fortran, and has been developed by Dr. G.A. Milne over a number of years in collaboration with Prof. J.X. Mitrovica at the University of Toronto (Milne 1998, Milne and Mitrovica 1998, Milne et al. 1999). The complete version of the code, which includes all of the advances described below, is used by a small user base of postgraduate students and postdoctoral researchers working in either Milne's or Mitrovica's research groups. The version of the code used for PSAR is the one described in Mitrovica and Milne (2003).

3.17.2 Suitability of the code

The GIA code solves the sea-level equation (Farrell and Clark 1976) via the pseudospectral approach developed by Mitrovica and Peltier (1991). The code has been significantly extended since this time to account for several different processes and thus improve the accuracy of the computation. Firstly, time-dependent shoreline positions are taken into account when calculating the ocean-loading function. Secondly, the water influx to regions vacated by retreating, marine-based ice is carefully accounted for in the distribution of the load (Milne et al. 1999). 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). These publications define the state-of-the-art in computing sea-level changes associated with glaciation.

A large part of the study with the GIA model (**Climate report** Section 3.3.4, Whitehouse 2009) was focused on selecting parameters (ice-load history and earth parameters) to enable detailed evaluation and validation of the model through sensitivity analysis and a case study. Some of the simulations were evaluated against today's patterns of isostatic uplift across Fennoscandia as observed by dGPS (Vestøl et al. 2019). Model validation showed, among other things, that GIA simulations in 3D, with laterally varying properties on the crust's thickness, gave results more in line with observed data, see **Climate report** Section 3.3.4 "A case study with a Fennoscandian 3D Earth structure". The size of the error introduced by the one-dimensional geometry, used in PSAR, is reported for Forsmark in the **Climate report** Section 3.3.4. The **Climate report** further reported that the uncertainty in the results of the GIA model is in some cases large (up to several tens of meters). This is summarized in **Climate report**, Section 3.3.7. Handling of uncertainties in SR-Site – Model simplification uncertainty. Therefore, the results from the GIA model of the relative sea-level change for the coming first 10 000 years is not used in SKB's climate scenarios. This period is instead based on other information.

The PSAR GIA model is used in a large number of studies on future changes in isostatic and sea-level response to global warming.

Although the evaluation of the model shows that the results may in some cases contain major uncertainties, the results were used in such a way that the model was appropriate for the issues that are relevant in the PSAR.

3.17.3 Usage of the code

Due to the nature of the development of the GIA code, and the intended user base, there is no formal documentation available. The correct usage of the code is assured since the numerical GIA model is used, since the SR-Site project, by scientists working in close collaboration with the developer of the code. The version used in PSAR 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 PSAR 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.

3.17.4 Development process and verification

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

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

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

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

3.17.5 Handling of input data, computational results and scripts

Data were transferred between the ice sheet (UMISM, see Section 3.23), GIA, and permafrost simulations (see Section 3.18) by text or Excel-files. Figure 3-3 shows the input and output data shared between the three models. Data are archived in SKBdoc 1927730 (Table 1-2).

3.17.6 Rationales for using the code in the PSAR

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

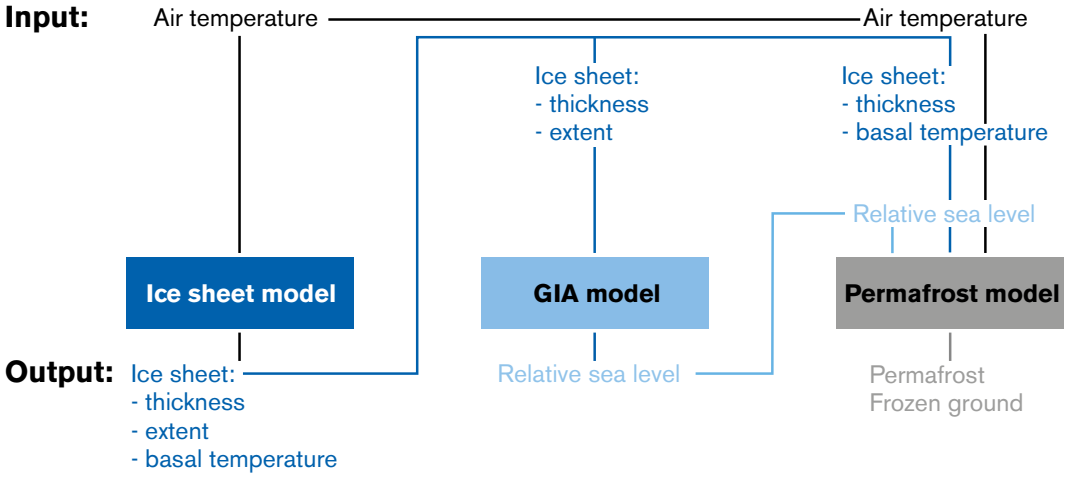

Figure 3-3. *Data transferred between the ice sheet (UMISM), GIA, and permafrost simulations.*

3.18 Numerical permafrost model

3.18.1 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 numerical 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 has been used in SR-Can (SKB 2006a) 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 simulations used in the PSAR the code was updated to deal with spatially varying surface conditions and salt transport as well as to solve large systems of equations. This 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, 2018). The study included features such as varying climate conditions, ground surface water bodies and topography, lateral variations in physical soil properties and heat generation from the spent fuel as well as effects of the phase change of saline water, groundwater flow and salt transport. The code is classified as a category 4b code.

3.18.2 Suitability of the code

The second version of the code, used in the PSAR, solves the equations of energy balance and mass balance of groundwater, ice and salts together with the generalized 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, 2018). The model, considering the ground as saline water saturated porous medium, 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 for glaciated periods, basal ice 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 stabilized bi-conjugate gradient algorithm (van der Vorst 1992) for the system of linearized equations.

Prior to the PSAR, the code has been used in several studies including soil freezing problems (Hartikainen and Mikkola 1997, 2006, Mikkola and Hartikainen 2001, 2002), and development of permafrost and perennially frozen ground (Hartikainen 2004, 2006, Chan et al. 2005, SKB 2006a).

3.18.3 Usage of the code

Description of the first version of the code is given in Freund and Lempinen (1994) and Hartikainen (1994, 2004), while the model settings for the second version of the code, as well as PSAR input and output data to the model, are described in Hartikainen et al. (2010).

3.18.4 Development process and verification

Validations of the numerical permafrost model used for simulation of permafrost and perennially frozen ground, salt extraction and impact on groundwater flow pattern were reported in Hartikainen et al. (2010, Section 3.6). The model was validated for i) density controlled groundwater flow (see Section 3.6.1 The Elder problem and Section 3.6.2 Salt fingering), ii) the effects of pressure and salinity at the groundwater temperature of the groundwater (see Section 3.6.3 Freezing point of saline water) , and (iii) salt freezing and salt transport in partially frozen soil (see Section 3.6.4 Uniaxial Freezing).

The validation of density-controlled groundwater flow showed that the model gave a slightly faster development of the salt concentration than the calculation model compared to the benchmark test with the Elder problem. The results further showed that the model yield results in good agreement with experimental observations of gravity driven convection of salt. Validation of the effects of pressure and salinity at the freezing temperature showed that the model generates data in very good agreement with experimental reference data. The validation of salt freezing also showed that the model produces data in accordance with large-scale laboratory tests.

The validations described above, along with the detailed and systematic management of uncertainties in the permafrost simulations, show that the permafrost model can be expected to provide useful results for the issues analysed in the PSAR.

In addition to the validation studies above, SKB plans to further validate the permafrost model by using the same version of the model used in SR-Site to simulate temperature bedrock, including permafrost and freezing depths, at the study area where SKB conducted the Greenland Analogue Project (GAP) in western Greenland (Claesson Liljedahl et al. 2016, Harper et al. 2016). Detailed direct observations show that permafrost today is just over 300 m deep at this site Data inputs for validation simulations (thermal properties of rock, chemical properties of groundwater, surface condition, climate, etc.) have been obtained from the GAP project and partly from published scientific literature, whereas input data in terms of Holocene air temperatures and Late Weichselian basal ice temperatures have been compiled and simulated for this study. Data against which the model will be validated (verical bedrock temperature distribution at the GAP-04 drillsite (Claesson Liljedahl et al. 2016)) comes from the GAP project.

3.18.5 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. Data transfer between the ice sheet (UMISM), GIA, and permafrost simulations is shown in Figure 3-3. MATLAB and COMSOL are used to pre- and post-process the data. Data are archived in SKBdoc 1927730 (Table 1-2).

3.18.6 Rationales for using the code in the PSAR

The code was selected for the SR-Site safety assessment and the PSAR since it is one of the world-leading in its field. The code was used in the PSAR for simulations of freezing of saturated bedrock for a reconstructing last glacial cycle conditions and for a large number of sensitivity tests.

3.19 PHAST

3.19.1 Introduction

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

In the SR-Site assessment, PHAST was used for modelling oxygen transport (melt water enriched in oxygen) during episodes of a glaciation cycle (Sidborn et al. 2010).

PHAST has also been used for the assessment of the interaction of the fully water-saturated bentonite with groundwater through a series of tree-dimensional (3D) numerical models (Sena et al. 2010a).

PHAST has also been used as numerical tool in previous performance assessment studies at 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).

The code is regularly updated. The code and revision history are available at (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phast/index.html). The latest version is PHAST v.2.0.2. Due to the frequent release of new revisions of the code, different versions of the code have been used, but most of the work performed in the SR-Site has been carried out using the version v.1.5.1.

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

3.19.2 Suitability of the code

PHAST is a robust geochemical code able to model the different geochemical processes of interest in the SR-Site assessment.

PHAST is a general computer code with the capability to model various reaction chemistry formulations (homogeneous equilibria using an ion-association thermodynamic model, heterogeneous equilibria between the aqueous solution and minerals, gases, surface complexation sites, ion exchange sites, solid solutions, and kinetic reactions). It can handle various equation-discretisation, types of boundary conditions (specified-head, flux and leaky conditions), source-sink, and equation-solver options. Four types of flow and reactive transport simulations can be performed with PHAST: steady-state simulation of groundwater flow, transient simulation of groundwater flow, steady-state simulation of flow followed by reactive transport and transient simulation of flow with reactive transport. PHAST is applicable to the study of natural and contaminated groundwater systems at a variety of scales ranging from laboratory experiments to local and regional field scales (Parkhurst et al. 2004). However, PHAST is not suitable for some types of reactive transport modelling, in particular for unsaturated zone flow, and simulating transport of gas phases and non-aqueous liquid phases. On the other hand, PHAST is restricted to constant temperature and density.

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

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

The aqueous model for PHAST is an ion-association model that is applicable to ionic strengths up to 1 molal. Thus, PHAST is not an appropriate simulator for many systems and processes, including transport of volatile organic compounds in a soil zone, hydrothermal systems, most high ionic-strength brines, or heat storage and recovery in aquifers. 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).

3.19.3 Usage of the code

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

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

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

3.19.4 Development process and verification

PHAST is a free geochemical modelling tool (non-commercial, open source), which is developed and maintained by the USGS (United States Geological Survey). It is relatively wide-spread, Google Scholar has more than 200 references that use, or cite, PHAST. Release notes available from the USGS website report changes between versions.

Verification of the code is included in the seven examples described in the manual (Parkhurst et al. 2010).

This type of reactive transport modelling tools is appropriate for fractured rocks (MacQuarrie and Mayer 2005) as well as for saturated bentonite-groundwater interactions (Arcos et al. 2003). Therefore, PHAST was adequate for its use in SR-Site, that is, modelling of oxygen ingress in granite fractures and modelling of water-saturated bentonite interaction with groundwater.

3.19.5 Handling of input data, computational results and scripts

All input and output files to PHAST are ASCII text files. Three types of input files are needed: a thermodynamic data base, described in the **Data report**, and two input files. One of them describes the initial composition of the aqueous solutions in each volume (for each material), and the mineral precipitation/dissolution reactions to be modelled. The other input file describes the grid, the transport parameters, including the time discretisation, and the boundary conditions.

For the modelling of oxygen intrusion along a fracture and into the rock matrix, the input files were created with a text editor. The output file, which consists of lines of text with column data, may be directly imported into other programs, such as Microsoft's Excel, for plotting.

The data used for modelling of oxygen ingress are archived at SKB (SKBdoc 1265689, see Table 1-2). The data used for modelling of bentonite – groundwater interaction are archived in SKBdoc 1265807 (Table 1-2).

3.19.6 Rationales for using the code in the PSAR

The assessment team has selected the PHAST code since it is useful to solve 3D fluid flow and reactive transport problems (advection, diffusion and dispersion) under water saturated conditions. The level of knowledge of this program is high and well-supported.

3.20 PHREEQC

3.20.1 Introduction

The PSAR post-closure safety assessment is based on the same set of PHREEQC calculations that supported the safety assessment SR-Site. PHREEQC is a free geochemical modelling tool (non-commercial, open source), which is developed and maintained by the USGS (United States Geological Survey). It is the culmination of a development policy initiated by the USGS in the sixties to develop geochemical tools. PHREEQC has become a modelling environment in which various modelling techniques have been introduced and improved that previously used to be separate USGS programs, including some of the most used in the eighties and nineties, such as WATEQ4F, PHREEQE and NETPATH.

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

It has been used for near-field (canister and the engineered systems) modelling activities in several ways. In some cases, it has been directly used to perform simple 1D transport modelling but in most cases has been used as a pre-conditioning tool for large scale 2D simulations performed with other codes. In SR-Site, it has been used for simulations of the evolution of the groundwater composition within the candidate repository site of the Forsmark and Laxemar areas assuming different climate conditions and hydrological situations. The hydrochemical calculations have been performed by simulating mixing of five end-member waters and mineral equilibrium reactions.

PHREEQC has been also used as numerical tool in previous performance assessment studies at SKB and elsewhere (Duro et al. 2006, Grivé et al. 2010a, Guimerà et al. 2006).

The version of the code is regularly updated. The code and revision history is available at (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/index.html). Due to the frequent release of new revisions of the code, different versions of the code have been used. However, most of the work performed has been carried out using PHREEQC v.2.10.

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

3.20.2 Suitability of the code

For the modelling of chemical behaviour at the candidate repository sites (Forsmark and Laxemar), under different climatic periods and hydrological assumptions, PHREEQC is a suitable tool. It can be used as a speciation program to calculate saturation indices as well as spatial and temporal distribution of aqueous species by mixing of solutions and considering equilibrium with mineral phases (including redox elements).

PHREEQC is based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, exchangers and sorption surfaces, but also includes the capability to model kinetic reactions with rate equations specified in the form of Basic statements. It also includes a 1D transport algorithm that comprises dispersion, diffusion and various options 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). Other limitation of the aqueous model is lack of internal consistency in the data in the databases. On the other hand, in reference to surface complexation calculations, PHREEQC incorporates the generalized two-layer model, a two-layer model that explicitly calculates diffuse-layer compositions, and a non-electrostatic surface-complexation model. Other models have not been implemented. With respect to solid solution simulations, ternary non-ideal solid solutions are not also implemented.

3.20.3 Usage of the code

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

Input data is easily introduced by means of the edit tool provided by the same program. Selected output data can be obtained in ASCII-text formatted files that can be read and modified with Microsoft Excel program or similar.

3.20.4 Development process and verification

Because it is so wide-spread, and due to the USGS's policy of constant maintenance and updating, there has been continuous feedback loop between users and developers: problems or errors have been detected quickly in new versions, resulting in quick and efficient corrections. This means that PHREEQC is possibly one of the more refined and widely used programs that currently exist. E.g. Google Scholar has more than 5000 references that use or cite PHREEQC. A confirmation that the program produces correct results is found in references that present comparisons of results between PHREEQC and other codes (De Windt et al. 2003, Gundogan et al. 2011, Nowack et al. 2006, Schüßler et al. 2001), as well as in some verification calculations reported in the user's manual. PHREEQC can be freely downloaded from the USGS website (June 14, 2013): http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/

On this website, under the heading "Status of PHREEQC Programs", a complete list of enhancements, changes and bug fixes that have been performed in the different versions of this code is available. The source is, therefore, public and completely and transparently traceable.

Therefore, SKB considers PHREEQC to be sufficiently verified for the purposes of SR-Site, i.e. equilibria in groundwater and with a few specific minerals. PHREEQC is adequate for such type of equilibrium and mixing calculations as evidenced in the manual and by the extensive number of peer-reviewed publications that use this code; a representative example is provided by Rebeix et al. (2011).

3.20.5 Handling of input data, computational results and scripts

All input and output files to PHREEQC are ASCII text files. Two types of input files are needed: a thermodynamic data base, described in the **Data Report**, 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.

For the modelling of the geochemical evolution of the groundwaters at Forsmark during a glacial cycle, simple computer programs were devised to create input files and to read and extract data from the output files. These programs and the procedure is described in detail in the Appendix of Salas et al. (2010). The output from the hydrogeological models, in terms of spatial coordinates, salinitities and, if available, mixing proportions of reference waters, together with the composition of these reference waters, was used to construct the input files to PHREEQC (Salas et al. 2010).

For the modelling of oxygen intrusion into the rock matrix, the format of an output file from PHREEQC ("selected output") is controlled through the input file. The selected output file, which consists of lines of text with column data, may be directly imported into other programs, such as Microsoft's Excel, for plotting.

The data used are archived at SKB (SKBdoc 1262945 and SKBdoc 1265689, see Table 1-2).

3.20.6 Rationales for using the code in the PSAR

The assessment team has selected the PHREEQC code because it is useful to characterize mixtures of solutions in equilibrium with mineral phases, considering simplistic 1D transport calculations, and for a high number of simulated points characterised by different mixing fractions. The level of knowledge of this program is high and well-supported.

3.21 Solubility model (Simple Functions)

3.21.1 Introduction

The Simple Functions spreadsheet is a tool to determine the solubility limits of radionuclides especially designed for Performance Assessment exercises. This tool has been developed for SKB in an Excel spreadsheet, and as such, it belongs to category 4b.

The development of this tool was promoted by the necessity of having a confident and easy-to-handle tool to calculate solubility limits in an agile and relatively fast manner. It was originally built up by Amphos 21 in the frame of the SR-Can project as a request by SKB. Later, it was improved by adding uncertainty calculation. For SR-Site, the tool was updated again (Grivé et al. 2010b) to incorporate recent thermodynamic data changes. Two versions are provided, which differ in the conditions under which the solubility assessment is done:

- VERSION A is designed to calculate radionuclide solubility limits in *representative groundwater compositions supplied by the user*.
- VERSION B is designed to calculate radionuclide solubility limits in a *groundwater that has interacted with Fe-corrosion products*.

Further work was performed to investigate the effects of including phosphate in the calculations (Grivé et al. 2013) Thus, another version of Simple Functions, which involves phosphate, is also available. The results show that not including phosphate results in higher solubility limits for some radionucildes.

3.21.2 Suitability of the code

This tool is an Excel spreadsheet that contains the simple algorithms needed to determine the solid phase that may exert the solubility control under the conditions of interest for a given radionuclide and its solubility.

The aim of the Simple Functions spreadsheet is to facilitate the calculation of the solubility limits. Current geochemical codes calculate the speciation of many different elements in solution, and use an associated thermodynamic database containing the stoichiometry and stability of every aqueous and solid species. Most of these thermodynamic databases are exhaustive, in an attempt to cover a wide range of water compositions and they contain information on aqueous species that only appear under very specific water compositions which have been judged to be of no interest for the current solubility assessment.

The Simple Functions spreadsheet is tailored for the conditions of interest and contains only those species accounting for at least 10 % of the total element in solution under the following range of conditions:

- $T = 25$ °C.
- $I \leq 0.2$ m (ionic strength (I) in molality units (m)).
- $6 < pH < 11$.
- $-8 < pe < 14$.
- $5 \times 10^{-5} < [SO_4] < 5 \times 10^{-2}$ (range of interest for SR-Site).
- $10^{-4} < [CO_3] < 5 \times 10^{-3}$ (range of interest for SR-Site).
- In VERSION A, $[Fe]_{aq}$ range given by the user; in VERSION B $[Fe]_{aq}$ is given by the equilibrium magnetite/goethite at the pH of interest.

The elements included in the Simple Functions spreadsheet are Sr, Ra, Ni, Sn, Se, Ag, U, Zr, Nb, Pa, Np, Pu, Am, Cm, Tc, Pd, Sm, Ho, Th and Pb. Moreover, the aqueous speciation of the following major elements is also considered: HCO_3^-, SO_4^{2-}, Cl^-, Ca^{2+}, Na^+ and Fe^{2+}.

Solubility limits for some radionuclides can vary with temperature. The effect of varying temperature between 0 and 90 °C has therefore been investigated by Grivé et al. (2013), who observed significant changes within that temperature range. The Simple Functions tool is tailored for scenarios where the temparures is around 25 °C. For scenarios where an elevated temperature is expected, the Simple Functions tool is not suitable without further temperature corrections.

3.21.3 Usage of the code

The capabilities of Simple Functions spreadsheet are described in the Simple Functions Spreadsheet tool presentation report (Grivé et al. 2010b). Input data are directly supplied into the Excel spreadsheet where the user can also find the output results.

This tool can be used together with the @RISK application (add-in to Microsoft Excel, see http://www.palisade.com/risk/) to perform probabilistic calculations.

3.21.4 Development process and verification

The Simple Functions spreadsheet has been developed as an easy-handling tool to calculate ranges and distributions of solubility limits to be used in the radionuclide transport calculations. Because of its simplicity, calculations are less complete than those used in other geochemical codes.

Simple Functions Spreadsheet tool presentation report (Grivé et al. 2010b) includes results of a benchmarking exercise in which the solubilities calculated with Simple Functions spreadsheet have been compared with the solubilities calculated with the code PHREEQC (Parkhurst and Appelo 2001) and in some cases calculated with the code HYDRA-MEDUSA (Puigdomenech 2002).

The validity of the activity correction approach used in the Simple Functions spreadsheet to calculate solubility values at high ionic strengths and the uncertainty associated with the Simple Functions spreadsheet calculations in the case of groundwater temperatures different from 25 °C (in the range 0 to 100 °C) have also been tested and reported in Grivé et al. (2010b).

The influence of temperature appears to be more important than that of the ionic strength, but in view of the results of the validation process, the Simple Functions spreadsheet can be considered a good tool for an easy and fast calculation of the solubility of radionuclides under the different groundwater compositions and temperatures of interest for SR-Site, always used with caution and keeping in mind its limitations.

Validation and sensitivity analysis activities during the development of Simple Functions are described in Chapter 4 of Grivé et al. (2010a). Solubilities calculated with Simple Functions are compared to those calculated with PHREEQC and HYDRA MEDUSA and the results are in good agreement.

Simple Functions is tailor made for the conditions and the near-field of interest, see Grivé et al. (2010b). How different sources of information, such as natural analogues, have been used to support the calculations and how uncertainties linked to solubility concentrations have been evaluated is also discussed in this reference. In Simple Functions, a few reasonable solubility limiting phases have been selected for each radionuclide. The selection of potential solubility limiting phases is done by expert judgement but based on thermodynamics. The process is described by Grivé et al. (2010) and Duro et al. (2006)

Duro et al. (2006) was written to support the safety assessment SR-Can and since then there have been changes in calculations of estimated solubilities. Therefore, the supplementary document (Grivé et al. 2010a), where updates are explained and assessed, were developed for SR-Site. The SR-Site version of Simple Functions (version B) is used also for the current assessment.

3.21.5 Handling of input data, computational results and scripts

The Simple Functions spreadsheet code is an Excel file. It is a user-friendly tool that requires the input of a groundwater composition and provides the concentration of radionuclides in equilibrium with their respective solubility limiting phases under the conditions of the groundwater composition. Therefore, any groundwater composition (calculated or measured) can be introduced in the tool. Calculated radionuclide concentrations can be directly used in other codes.

In SR-Site, groundwater data is supplied to the tool, which contains the uncertainties in thermodynamic data for the relevant reactions. The output produced is the solubility limit for the radioelements. Together with the @RISK tool, Simple Functions is used to calculate distributions of solubility to be used in the radionuclide transport calculations in SR-Site. Additional information regarding this method is provided by Sellin et al. (2013).

The data used are archived at SKB (SKBdoc 1265616, see Table 1-2).

3.21.6 Rationales for using the code in the PSAR

The assessment team has selected the Simple Functions Spreadsheet since it is a tailor-made tool for the production of probabilistic distributions of radioelement solubilities. The results produced by the tool are in good agreement with those from conventional geochemical codes (e.g. PHREEQC).

3.22 TOUGHREACT

3.22.1 Introduction

The PSAR post-closure safety assessment is based on the same set of TOUGHREACT calculations that supported the safety assessment SR-Site.TOUGHREACT is a widely used commercial code developed at the Lawrence Berkeley National Laboratory (LBNL). TOUGHREACT is used in SR-Site for simulations of reactive transport in the buffer (Sena et al. 2010a).

TOUGHREACT v.1.2 (Xu et al. 2008) results from coupling the calculation of geochemical reactions to the TOUGH2 code (Pruess et al. 1999), which solves multiphase, non-isothermal fluid flow, heat flow and multi-component transport. Aqueous complexation, gas dissolution/ex-solution and cation exchange are modelled under local equilibrium. Mineral precipitation/dissolution may be modelled either under equilibrium or kinetics assumptions. Additionally, changes in porosity, permeability and capillary pressure may be computed (Pruess et al. 1999).

TOUGHREACT has been used by SKB in the “SKB-NF-2009” (Sena et al. 2010a) and “LOT-A2 experiment” (Sena et al. 2010b) projects. In the project “LOT-A2 experiment”, a 1D axis-symmetric model was developed to simulate the thermo-hydraulic, transport and geochemical processes that have been observed during the LOT A2 test. In the SKB-NF-2009 project, the effect of the thermal period and the water saturation are analysed. These simulations are based on the outcomes of the previous numerical model built for the simulation of the LOT-A2 experiment.

Since the code is not written exclusively for SKB projects, the code is regarded as a category 3 code.

3.22.2 Suitability of the code

The first version of the code was developed by introducing reactive geochemistry into the framework of the existing multi-phase fluid and heat flow code TOUGH2 (Pruess 1991). The present version of TOUGHREACT provides the following equation-of-state modules: EOS1, with typical applications to hydrothermal problems, EOS2 for multiphase mixtures of water and CO_2 with typical applications to hydrothermal problems, EOS3 for multiphase mixtures of water and air with typical applications to nuclear waste disposal problems, EOS4 with the same capabilities as EOS3 but with vapour pressure lowering effects due to capillary pressure, EOS9 with typical applications to ambient temperature and pressure reactive geochemical problems, and ECO2N for multiphase mixtures of water, CO_2 and NaCl with typical applications to CO_2 disposal in deep brine aquifers. TOUGHREACT is appropriate for this type of models as described in its documentation and several publications, for example Itälä et al. (2011) and Arthur and Zhou (2005).

More detailed information on the geochemical and fluid flow and transport equations solved can be obtained from the TOUGHREACT User's Guide (Xu et al. 2008) and the TOUGH2 User's Guide, version 2.0 (Pruess et al. 1999).

3.22.3 Usage of the code

In the TOUGHREACT User's Guide (Xu et al. 2008) different examples have been included as test problems (geothermal systems, diagenetic and weathering processes, subsurface waste disposal, acid mine drainage remediation, contaminant transport and groundwater quality). The major processes for fluid and heat flow are: (1) fluid flow in both liquid and gas phases under pressure, viscous and gravity forces, (2) interactions between flowing phases represented by characteristic curves (relative permeability and capillary pressure), (3) heat flow by conduction and convection, and (4) diffusion of vapor and air (Pruess et al. 1999). Aqueous complexation, acid-base, redox, gas dissolution/ex-solution, and cation exchange are considered under local equilibrium. Mineral dissolution and precipitation can proceed either subject to local equilibrium or kinetic conditions (Xu et al. 2008). Linear adsorption and decay can be included.

3.22.4 Development process and verification

The code was developed by the Earth Sciences Division of the Lawrence Berkeley National Laboratory (University of California) as a comprehensive non-isothermal multi-component reactive fluid flow and geochemical transport simulator to be applied to many geologic systems and environmental problems. 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. Gundogan et al. (2011), Pruess et al. (2004) and Xu et al. (1999) describe either the verification, or inter-code comparison of TOUGHREACT.

3.22.5 Handling of input data, computational results and scripts

Input data and output results are easily treated by means text editors. Output data can be also easily selected and obtained in .txt or .dat files that can be read and modified with Microsoft Excel program or similar.

Three input files are required: (1) flow.inp, including rock properties, time-stepping, grid, initial and boundary conditions and data related to a multi-phase fluid and heat transport simulations (Pruess et al. 1999); (2) solute.inp, containing flags and input parameters for reactive transport calculations (diffusion coefficients, tolerances, e.g.); and (3) chemical.inp, defining the geochemical system, initial water compositions, material zones, and kinetic data for minerals. In addition, the program requires a thermodynamic database file.

The data used are archived at SKB (SKBdoc 1265618, see Table 1-2).

3.22.6 Rationales for using the code in the PSAR

The assessment team has selected the TOUGHREACT code because it is useful to solve non-isothermal and multicomponent reactive fluid flow and geochemical transport calculations. The level of knowledge of this program is high and well-supported.

3.23 UMISM

3.23.1 Introduction

UMISM (University of Maine Ice Sheet Model) is a 3D thermo-mechanical ice-sheet model capable of simulating realistic ice sheets that are typically not in balance with climate (advances and retreats given changes in external forcing).

UMISM is used in PSAR for reconstructing the ice sheet of the last glacial cycle in order to construct the reference glacial cycle, 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 the Fennoscandian ice sheet for various purposes (e.g. Fastook and Holmlund 1994, Holmlund and Fastook 1995, Näslund et al. 2003) and in SKB safety assessments (SKB 2006a, 2008, 2010c).

The UMISM finite-element code (Fortran) was originally developed by Prof. J. Fastook, at the Computer Science Department 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 PSAR, the version of UMISM as of October 2004/April 2005 was used. The code is classified as a category 4b code.

3.23.2 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. The mass balance is determined from an empirical relationship constituting a simple parameterisation of the ice sheet's effect on local climate (Fastook and Prentice 1994). Distributed air temperatures over the model domain are determined from height over sea level and distance from the pole. The UMISM model includes a mathematical description of precipitation from a number of other parameters; distance from the pole, saturation vapour pressure (function of altitude and laps-rate), and surface slope. This is an empirical relationship developed from the Antarctic ice sheet (Fastook and Prentice 1994). Over a certain model domain, with a topography described from a Digital Elevation Model (DEM), this climate description gives a spatial pattern of air temperatures at ground level and a pattern of precipitation. Given a suitable climate forcing, the model develops a thermomechanical 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.

3.23.3 Usage of the code

In the PSAR ice sheet reconstruction simulations, inputs 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 these runs, the program simulates the 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., text format or NetCDF (Network Common Data Form) format.

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

3.23.4 Development process and verification

As discussed in the **Climate report,** Section 3.1.14, the UMISM model has previously been validated against other ice-sheet models of the same type, i.e. other thermo-mechanical ice sheet models, as a part of the EISMINT (European Ice Sheet Modelling Initiative) model intercomparison project. The results showed that UMISM results comply well with these other models (Huybrechts et al. 1996, Payneet al. 2000). The model uncertainties that the version of UMISM used in SR-Site contained was reported in **Climate report,** Section 3.1.7.

For the PSAR, the ice sheet model was capable of producing a general development of the Weichselian ice sheet which complies with the overall Weichselianglacial history as known from quaternary geology, glacial morphology, etc. studies (**Climate report**, Section 4.2). In addition, the model produced a

development of the ice sheet during mid-Weichselian with a very limited size of the ice sheet. This was not the common picture of the Weichselian glacial history at the time of the simulation (2005), but later proved to be correct through new quaternary geological studies in Scandinavia, see **Climate report,** Section 4.2, and rferences therein.

In addition, the model also provides similar results as a result of completely different types of ice sheet models (Dick Peltiers ICE-5G and Kurt Lambeck's ANU), which are based on another methodology (isostatic response and resulting ice load history) (see Schmidt et al. 2014).

All in all, UMISM is expected to provide useful results for the approach that SKB has chosen to use for climate and climate-related issues, including effects of glaciation.

3.23.5 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 PSAR activities, such as the permafrost modelling (Hartikainen et al. 2010 and **Climate report**, Section 3.4), Global Isostatic Adjustment (GIA) modelling conducted at University of Durham by P. Whitehouse (**Climate report**, Section 3.3), and for modelling of crustal stresses performed at university of Uppsala performed by B. Lund (Lund et al. 2009). How data is transferred between the ice sheet (UMISM), GIA, and permafrost simulations is shown in Figure 3-3.

Output data were transferred from the UMISM model to other PSAR activities in text files and Excel spread sheets. Output data are archived in SKBdoc 1927730 (Table 1-2).

3.23.6 Rationales for using the code in the PSAR

The UMISM code was selected for the PSAR safety assessment since several simulations of the Fennoscandian ice sheet have been done 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, which is highly relevant for the PSAR safety assessment. An additional reason for choosing this model is the recognized ability and interest of the model developer to engage in validating and assessing model results against real-world observations and phenomena related to the ice sheet system that is being modelled. This is important in phases of model calibration as well as when adopting and developing the model to specific needs of the project.

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