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Post-closure safety for SFR, the final repository for short-lived radioactive waste at Forsmark

Model tools summary report, PSAR version

SVENSK KÄRNBRÄNSLEHANTERING AB

SWEDISH NUCLEAR FUEL
AND WASTE MANAGEMENT CO

Box 3091, SE-169 03 Solna
Phone +46 8 459 84 00
skb.se

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Summary

This report describes computer codes used in modelling studies for the post-closure safety assessment in PSAR SFR. The PSAR assessment of post-closure safety is an important part of the construction license application for the extension of SFR. This report constitutes one of the main references supporting the **Post-closure safety report.** The aim of this report is to document the quality assurance (QA) processes associated with each code according to the description given in chapter two.

The models applied in post-closure safety assessment vary significantly in terms of their complexity, and some codes are commercial, whereas others were developed, or adapted, for SKB assessments. To account for the diversity of the codes, the following QA reporting requirements were identified:

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

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

Sammanfattning

Denna rapport beskriver de olika datorkoder som använts inom analysen av säkerhet efter förslutning i PSAR SFR. Analysen av säkerhet efter förslutning i PSAR är en viktig del av ansökan om medgivande för utbyggnaden av SFR. Denna rapport utgör en av huvudreferenserna till **Huvudrapporten säkerhet efter förslutning.** Syftet med rapporten är att dokumentera kvalitetssäkringen av koderna enligt den metodik som anges i andra kapitlet.

Beräkningskoderna som används inom analysen för säkerhet efter förslutning varierar mellan allt från kommersiella datorprogram till program specifikt utvecklad för SKB:s säkerhetsanalyser. Detta ställer olika krav på kvalitetssäkringsmetodiken. Följande krav på varje kod identifierades:

- Visa att koden är lämplig för det den är avsedd för.
- Visa att koden kan användas på ett korrekt sätt, det vill säga att koden är tillräckligt dokumenterad.
- Visa att koden har programmerats och utvecklats på ett korrekt sätt och att den ger korrekta resultat.

Även om kraven är identiska för alla koder, är de åtgärder som används för att visa att dessa krav har uppfyllts olika för olika koder. Varje enskild kod presenteras därför tillsammans med en diskussion om hur dessa krav uppfylls.

Contents

1 Introduction

This document is one of the main references to the **Post closure safety report** that contributes to the preliminary safety analysis report (PSAR) for SFR, the repository for short-lived low- and intermediate-level radioactive waste in Forsmark in Östhammar municipality.

This chapter gives the background and a short overview of the PSAR post-closure safety assessment undertaken as part of a stepwise license of the extension of SFR. Moreover, the purpose and content of this report is described.

1.1 Background

SFR is operated by the Swedish Nuclear Fuel and Waste Management Company, SKB, and is part of the Swedish system for management of waste from nuclear power plants, other nuclear activities, industry, research and medical care. In addition to SFR, the Swedish nuclear waste management system also includes the repository for spent nuclear fuel and the repository for long-lived radioactive waste (SFL).

SFR consists of the existing part, SFR1 (Figure 1-1, grey part), and the extension, SFR3 (Figure 1-1, blue part). SFR1 is designed for disposal of short-lived low- and intermediate-level waste produced during operation of the Swedish nuclear power reactors, as well as waste generated during the application of radioisotopes in medicine, industry, and research. This part became operational in 1988. SFR3 is designed primarily for disposal of short-lived low- and intermediate-level waste from decommissioning of nuclear facilities in Sweden. The extension is called SFR3 since the name SFR2 was used in a previous plan to build vaults adjacent to SFR1. The repository is currently estimated to be closed by year 2075.

The SFR waste vaults are located below the Baltic Sea and are connected to the ground surface via two access tunnels. SFR1 consists of one 70-metre-high waste vault (silo) and four 160-metre-long waste vaults (1BMA, 1–2BTF and 1BLA), covered by about 60 metres of bedrock. SFR3 consists of six waste vaults (2BMA, 1BRT and 2–5BLA), varying in length from 255 to 275 m, covered by about 120 metres of bedrock.

A prerequisite for the extension of SFR is the licensing of the extended facility. The licensing follows a stepwise procedure. In December 2014, SKB submitted two licence applications to extend and continue the operation of SFR, one to the Swedish Radiation Safety Authority (SSM) for permission under the Act on Nuclear Activities (SFS 1984:3) and one to the Land and Environment Court for permissibility under the Environmental Code (SFS 1998:808). In October 2019 SSM submitted their pronouncement to the Swedish Government and recommended approval of the permission sought by SKB. In November 2019 the Court submitted its statement to the Swedish Government and recommended approval of the licence application. The Swedish Government granted permit and permissibility in December 2021.

The current step in the licensing of the extended SFR is the processing of the construction license application, submitted by SKB to SSM for review under the Act on Nuclear Activities. The licence documentation consists of an application document and a set of supporting documents. A central supporting document is the preliminary safety analysis report (PSAR), with a general part consisting of ten chapters[1]. Chapter 9 of the general part of that report addresses post-closure safety. The **Post-closure safety report** is the main reference to Chapter 9, and this report is a main reference to the **Post-closure safety report**.

[1] SKB, 2022. PSAR SFR – Allmän del kapitel 1 – Introduktion. SKBdoc 1702853, (ver 3.0), Svensk Kärnbränslehantering AB. (In Swedish.) (Internal document.)

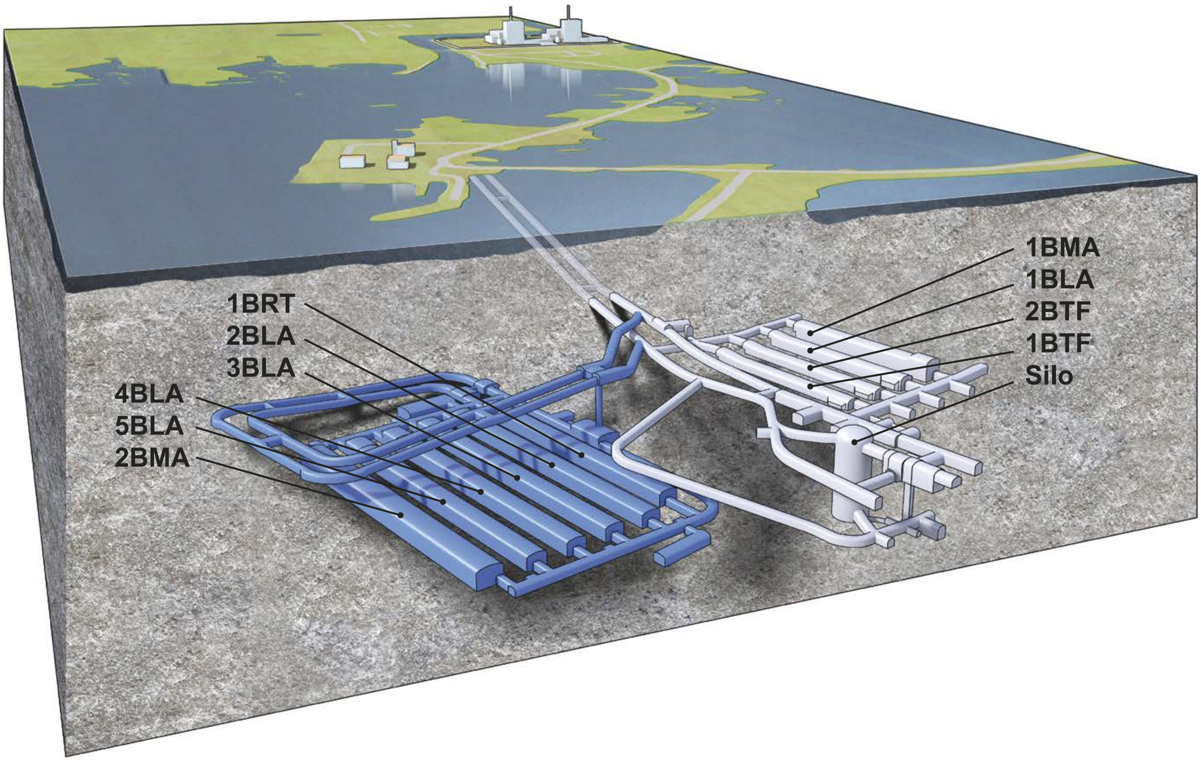

Figure 1-1. *Schematic illustration of SFR. The grey part is the existing repository (SFR1) and the blue part is the planned extension (SFR3). The waste vaults in the figure are the silo for intermediate-level waste, 1–2BMA vaults for intermediate-level waste, 1BRT vault for reactor pressure vessels, 1–2BTF vaults for concrete tanks and 1–5BLA vaults for low-level waste.*

1.2 Post-closure safety assessment

1.2.1 Overview

The main role of the post-closure safety assessment is to demonstrate that SFR is radiologically safe for humans and the environment after closure. This is done by evaluating compliance with respect to the Swedish Radiation Safety Authority's regulations concerning post-closure safety and the protection of human health and the environment. Furthermore, the post-closure safety assessment is being successively developed in the stepwise licensing process for the extended SFR, and thus the results from the PSAR assessment[2] provide input to the forthcoming updated assessment to be carried out before trial operation of the facility.

The overall aim in developing a geological repository for nuclear waste is to ensure that the amounts of radionuclides reaching the accessible biosphere are such that possible radiological consequences are acceptably low at all times. Important aspects of the regulations are that post-closure safety shall be maintained through a system of passive barriers. The barrier system of SFR comprises engineered and natural barriers and the function of each barrier is to, in one or several ways, contribute to the containment and prevention or retention of dispersion of radioactive substances, either directly or indirectly by protecting other barriers in the barrier system. To achieve post-closure safety, two safety principles have been defined. *Limitation of the activity of long-lived radionuclides* is achieved by only accepting waste for disposal that conforms with the waste acceptance criteria for SFR. *Retention of radionuclides* is achieved by the function of the engineered and natural barriers. The two safety principles are interlinked and applied in parallel. The engineered barrier system is designed for an inventory that contains a limited amount of long-lived radionuclides, given the conditions at the selected site and the natural barriers.

[2] For brevity, the PSAR post-closure safety assessment for SFR is also referred to as "the PSAR assessment" or "the PSAR" in the present report.

The basis for evaluating compliance is a safety assessment methodology that conforms to the regulatory requirements regarding methodology, and that supports the demonstration of regulatory compliance regarding post-closure safety and the protection of human health and the environment. The overall safety assessment methodology applied is described in the **Post-closure safety report**, Chapter 2. The methodology was developed in SR-PSU (SKB TR-14-01[3]) based on SKB's previous safety assessment for SFR1 (SAR-08, SKB R-08-130). Further, it is consistent with the methodology used for the post-closure safety assessment for the final repository for spent nuclear fuel to the extent appropriate given the different nature of the two repositories.

1.2.2 Report hierarchy

The **Post-closure safety report** and main references for the post-closure safety assessment are listed and briefly described in Table 1-1, also including the abbreviated titles (in bold) by which they are identified in the text. Furthermore, there are numerous additional references that include documents compiled either by SKB or other organisations, or that are available in the scientific literature, as indicated in Figure 1-2.

Table 1-1. Post-closure safety report and main references for the post-closure safety assessment. The reports are available at www.skb.se.

Abbreviated title by which the reports are identified in this report and in the main references **Report number**	**Content**
Post-closure safety report SKB TR-23-01	The main report of the PSAR post-closure safety assessment for SFR.
Initial state report SKB TR-23-02	Description of the expected conditions (state) of the repository at closure. The initial state is based on verified and documented properties of the repository and an assessment of its evolution during the period up to closure.
Waste process report SKB TR-23-03	Description of the current scientific understanding of the processes in the waste form and in the packaging that have been identified in the FEP processing as potentially relevant for the post-closure safety of the repository. Reasons are given as to why each process is handled in a particular way in the safety assessment.
Barrier process report SKB TR-23-04	Description of the current scientific understanding of the processes in the engineered barriers that have been identified in the FEP processing as potentially relevant for the post-closure safety of the repository. Reasons are given as to why each process is handled in a particular way in the safety assessment.
Geosphere process report SKB TR-14-05	Description of the current scientific understanding of the processes in the geosphere that have been identified in the FEP processing as potentially relevant for the post-closure safety of the repository. Reasons are given as to why each process is handled in a particular way in the safety assessment.
Climate report SKB TR-23-05	Description of the current scientific understanding of climate and climate-related issues that have been identified in the FEP processing as potentially relevant for the post-closure safety of the repository. Description of the current scientific understanding of the future evolution of climate and climate-related issues.
Biosphere synthesis report SKB TR-23-06	Description of the present-day conditions of the surface systems at Forsmark, and natural and anthropogenic processes driving the future development of those systems. Description of the modelling performed for landscape development, radionuclide transport in the biosphere and potential exposure of humans and non-human biota.
FEP report SKB TR-14-07	Description of the establishment of a catalogue of features, events and processes (FEPs) that are potentially relevant for the post-closure safety of the repository.
FHA report SKB TR-23-08	Description of the handling of inadvertent future human actions (FHA) that are defined as actions potentially resulting in changes to the barrier system, affecting, directly or indirectly, the rate of release of radionuclides, and/or contributing to radioactive waste being brought to the surface. Description of radiological consequences of FHAs that are analysed separately from the main scenario.

[3] For SKB reports without named authors, the report number is used instead of publication year when referring to them in the text.

Abbreviated title by which the reports are identified in this report and in the main references Report number	Content
Radionuclide transport report SKB TR-23-09	Description of the radionuclide transport and dose calculations carried out for the purpose of demonstrating compliance with the radiological risk criterion.
Data report SKB TR-23-10	Description of how essential data for the post-closure safety assessment are selected, justified and qualified through traceable standardised procedures.
Model tools report SKB TR-23-11 (this report)	Description of the model tool codes used in the safety assessment.

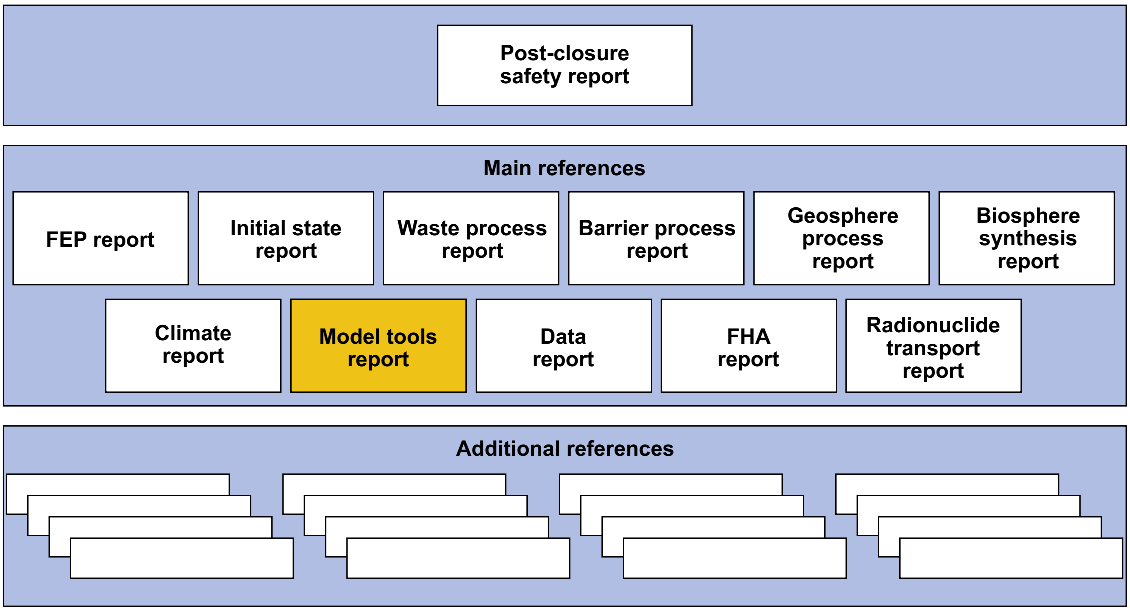

Figure 1-2. *The hierarchy of the Post-closure safety report, main references and additional references in the post-closure safety assessment.*

1.3 This report

1.3.1 The role of this report in the post-closure safety assessment

The ten steps in the methodology applied to assess post-closure safety for SFR are described in Chapter 2 of the **Post-closure safety report**. The steps are carried out partly concurrently and partly consecutively. This report gives an overview of the computer codes used in modelling activities performed in support of the following steps of the methodology:

Step 2: Description of the initial state for the analysis, defined as the expected state of the repository and its environment at closure.

Step 3: Description of external conditions, including climate and climate-related issues relevant for the future evolution of the repository and its environs.

Step 4: Description of internal processes.

Step 7: Description of the probable post-closure evolution of the repository and its environs (the reference evolution), i.e. a range of probable future evolutions of the repository and its environs.

Step 9: Selection and analysis of scenarios, each scenario describing a sequence of events and conditions of the repository and its environs and how they affect the protective capability of the repository.

1.3.2 Purpose of this report

A large number of computer codes have been used in different modelling activities to analyse post-closure safety. The models applied vary significantly in terms of complexity. Some of the applied codes are commercial, whereas others have been developed or modified to SKB´s specific needs. The purpose of the report is to document the quality assurance (QA) procedures and documentation relating to each code. This includes demonstrating that the code is suitable for its purpose, that it can be properly used and, when applicable, that the development process has followed appropriate procedures and the code provides accurate results.

This report is an update of the model summary report for the safety assessment SR-PSU (SKB TR-14-11). The extent of the update is described in Section 1.3.3 and the contributing experts in Section 1.3.4.

1.3.3 Main developments since SR-PSU

The model summary report for the SR-PSU gave an overview of both the modelling activities and computer codes used in post-closure safety assessment and quality assurance procedures and documents relating to the codes. The report included an assessment model flow chart (AMF) that described the modelling activities and how the different activities were connected. In the PSAR, the AMF is separated from the quality assurance procedures relating to the computer codes. The present report focuses on the latter, whereas the AMF is included in the **Main report**.

1.3.4 Contributing experts

Project leader for the PSAR safety assessment has been Jenny Brandefelt (SKB). The editor of this report has been Teresita Morales (SKB). In addition, a number of people from various fields of expertise have been involved in the development of models as well as the verification and descriptions of model codes, based on the model summary report for SR-PSU.

This report has been significantly improved at different stages by adjustments in accordance with comments provided by the contributing experts and the factual reviewers Fredrik Vahlund (SKB) and Mike Thorne (Mike Thorne and Associates Ltd.).

1.4 Structure of this report

This report comprises three chapters. The following is a brief description of the contents:

Chapter 1 – **Introduction.** This chapter describes the background and the role of the report.

Chapter 2 – **Quality assurance principles for the computer codes**. This chapter describes the quality assurance principles relating to the computer codes used in the post-closure safety assessment. Different categories of computer code are defined, and the QA requirements are given for each category. Finally, a template for describing the different codes is presented and further applied in Sections 3.1 to 3.15.

Chapter 3 – **Description of the codes**. This chapter provides descriptions of codes used in modelling activities included in the post-closure safety assessment in the PSAR SFR, following the template given in Section 2.3. In general, the modelling performed for SR-PSU is also included as a basis for the PSAR.

Appendix A – Terms and abbreviations. This appendix contains descriptions of terms and abbreviations used in this report.

2 Quality assurance principles for the computer codes

This chapter describes the quality assurance principles relating to the computer codes used in the post-closure safety assessment. Different categories of computer code are defined and the QA requirements are given for each category. Finally, a template for describing the different codes is presented and further applied in Sections 3.1 to 3.15.

2.1 Types of codes used in the assessment

A large number of codes are used within modelling activities to support the post-closure safety assessment. The different codes use a range of complex to simple routines written in various ways ranging from scripts embedded in commercially available codes such as MATLAB or Microsoft Excel, to larger programs written in programming languages such as C++ and FORTRAN. The origins of the codes also differ substantially; some are commercial, have a large world-wide user base and can be regarded as well tested, whereas others were written exclusively for SKB's post-closure safety assessments. The source codes developed for SKB's post-closure safety assessments are generally available for review, whereas the quality assurance procedures of the developer of commercial codes generally need to be accepted. Hence a differentiated approach of quality assurance, with adaptations to the types of codes used and developed within the post-closure assessment, is required.

The following categories of computer codes have been identified:

1. **Commercial system software** such as operating systems, compilers and database software. Although necessary for the post-closure safety assessment, these codes are not regarded as assessment codes and are hence not included in the current report.

2. **Software used to solve problems that can be verified by simple calculations**. This category also includes codes used for unit conversion and pre- and post-processing of data. This category is not included 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. Verification tests within the post-closure safety assessment are hence not warranted. These codes are not written exclusively for the safety assessment and the user of the code may in many cases be an expert on using the code. The documentation for these codes is generally extensive but may not be written with any specific application in mind. Source codes for commercial software are generally not available for review and the development process will have been carried out independently of the post-closure safety assessment. 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, there is a greater need for verification studies for these codes than for codes in category 3. 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 such as C++ and FORTRAN. In general, these codes are written with the safety assessment application in mind and have a considerably smaller user base than codes in category 3. There is therefore a greater need for verification and for the implementation of quality assurance procedures for these codes.

There may be cases where it is not evident whether a code belongs to category 4a or 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.

Based on these, above mentioned categories, the quality assurance procedures for each type of code are presented in Section 2.2.

2.2 Requirements for assessment codes

There are three basic requirements for the quality assurance of each code:

1. The code is suitable for its purpose – required for all categories.
2. The code can be properly used, i.e. the code is sufficiently documented – required for all categories.
3. The code development process has followed appropriate procedures and the code produces accurate results – this applies to category 4 codes because these have been developed by the implementer. For codes in categories 1–3, the procedures used by the developer are accepted.

The requirements are described further in Section 2.3, within the template for reporting the codes in the present report.

2.3 Template used for reporting the codes in Chapter 3

2.3.1 Introduction

The code is briefly introduced and its categorisation, made according to the definitions in Section 2.1, is given. In support of verification of the suitability of the code for its purpose, this section contains the following:

- A brief description of problems that can be solved by the code.
- A brief description of problems solved by the code in SKB's post-closure safety assessments.
- If the code was used in the previous safety assessment (SR-PSU) for SFR 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 definitions 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.

2.3.2 Documentation of the code

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

- A description or references to supporting documents of the mathematical models used (the equations to be solved) and a description of the methods by which the solution is obtained.
- A description or references to supporting documents of usage of the code (user's manual).

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

2.3.3 Development process and verification

For codes that have been developed for SKB's post-closure safety assessments (category 4), it needs to be shown that the development process has been carried out in an appropriate manner. This section is required to contain the following:

- The measures that have been taken to ensure that the code produces the correct solution to the mathematical problem. This can, for example, be achieved by comparison to solutions obtained with other codes or to analytic solutions for special cases.

- A description of how consistency 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 across the range of contexts in which it is to be applied.

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

2.3.4 Rationale for using the code in the assessment

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

3 Description of the codes

This chapter provides descriptions of codes used in modelling activities included in the post-closure safety assessment in the PSAR for SFR, following the template given in Section 2.3. In general, the modelling performed for the SR-PSU is also included as a basis for the PSAR.

3.1 3DEC

3.1.1 Introduction

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

3DEC was originally developed for stability analyses of fractured rock slopes. It has been used for studies related to mining engineering and for studies related to deep disposal of nuclear waste. Both static and dynamic analyses for deep underground openings have been performed, see for instance Stephansson et al. (1991), Sjöberg (1992) and Senseny (1993). 3DEC has been used by SKB in earlier studies regarding thermo-mechanical effects on the bedrock around a KBS-3 type of repository (Hakami et al. 1998). In SR-Can and SR-site, 3DEC was used for static analyses of mechanical effects on rock and rock fractures within and around the repository (Fälth and Hökmark 2007, Hökmark et al. 2010), and for dynamic analyses of fracture shear displacements induced by postglacial fault movements (Fälth and Hökmark 2006, Fälth et al. 2010). 3DEC is currently used by engineers, consultants and researchers in more than 30 countries around the world.

For the SR-PSU, 3DEC was used to carry out 3D numerical analyses of the stability of the SFR rock vaults after excavation and over the following 10 000 years (Mas Ivars et al. 2013). The model examined rock fallout and the stability of the rock pillar between waste vaults. The modelling performed for the SR-PSU is also included as a basis for the PSAR.

The SR-PSU 3DEC analyses were run on Windows-based PC-systems using 3DEC version 4.20 (Itasca 2011). 3DEC is a commercial code with a large user base, and so is a category 3 code.

3.1.2 Documentation of the code

The documentation of 3DEC (Itasca 2003, 2007, 2011) is provided with the software installation package by Itasca Consulting Group Inc. and may also be available at the Itasca Website: https://www.itascacg.com/software/3dec-software-documentation.

The documentation contains a complete description of the code and the constitutive models that are implemented.

All input and output data (geometries, material data, initial- and boundary conditions, solution strategies) are entered or exported as text files. 3DEC has a graphical user-interface that facilitates the process of building the model (geometry, application of boundary conditions etc). The user interface also has a wide range of possibilities for producing vector- and contour plots for post-processing and presentation of the results.

3.1.3 Development process and verification

The formulation and development of the distinct element method, which is the core of 3DEC, begun in 1971 (Cundall 1971) and has been on-going since then. The 3DEC documentation includes a suite of systematic comparisons between 3DEC results and corresponding analytical solutions. Models with different types of geometry, different types of material behaviour and different types of boundary conditions are included. The documentation can be accessed at the Itasca Website: http://www.itascacg.com/software/3dec.

3.1.4 Rationales for using the code in the assessment

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

3.2 ADINA

3.2.1 Introduction

The ADINA software (ADINA 2010) is a finite element program designed for statics and dynamic stress analysis of solids and structure (2D and 3D). The program implements finite element models to solve these stress analysis problems and is used within many different industries. The analysis can be linear or highly nonlinear, including effects of material nonlinearities, large deformations and contact conditions.

ADINA version 8.9.1 running on Windows 7 was used in the SR-PSU to estimate the strength of the barriers of the Silo in SFR1 earthquake events of different magnitudes and hence different frequencies of occurrence. The aim was to find the critical load and at what probability level the integrity of the structure may be compromised. Assumptions and simplifications made in the modelling and analysis phases are presented in Georgiev (2013). The modelling performed for the SR-PSU is also included as a basis for the PSAR.

Since ADINA is widely used commercial software with a large user base it is classified as a category 3 code.

3.2.2 Documentation of the code

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

The software modelling is performed by solving a large system of partial differential equations arranged in a finite element model mesh grid reflecting the geometry of the system. All input and output files to ADINA are ASCII text files that can be read and modified with standard tools. All the equations are given in Georgiev (2013, Appendix A).

3.2.3 Development process and verification

ADINA is commercial software developed by American company ADINA R&D. The code is widely used and its algorithm has been checked in several scientific publications (see ADINA website http://www.adina.com) and through the example files distributed with the computer program.

3.2.4 Rationales for using the code in the assessment

The ADINA code was selected for the post-closure safety assessment since it can model stress analysis using the finite element method. The program is widely used, well suited to nuclear waste disposal scenarios and well supported.

3.3 ArcGIS

3.3.1 Introduction

ESRI's ArcGIS is a geographic information system (GIS) used for creating and using maps, compiling geographic data, and analysing spatial distributed information. It uses maps and geographic information in a range of applications and manages geographic information in a database. ArcGIS has been used as a supportive tool in several fields.

ArcGIS was used in the SR-PSU for terrain and landscape development models. Two versions, ArcGIS 9.3 and ArcGIS 10.2 were used, on Windows XP and Windows 7 platforms respectively. Specifically, it constituted the main modelling tool when developing the digital elevation model (DEM), the vegetation model and the regolith models (**Biosphere synthesis report**, Strömgren and Brydsten 2013, Sohlenius et al. 2013). ArcGIS was also used in the landscape modelling, describing the past, present and future landscape in Forsmark in terms of land use and shoreline displacement (**Biosphere synthesis report**, Brydsten and Strömgren 2013). The modelling performed for the SR-PSU is also included as a basis for the PSAR.

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

3.3.2 Documentation of the code

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

3.3.3 Development process and verification

The ArcGIS code is a commercial geographic information system (GIS) code that is developed by ESRI. In 1999 ArcGIS 8.0 was released, replacing the previous software version from ESRI; ArcView.

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

3.3.4 Rationales for using the code in the assessment

ArcGIS is a well-established tool that is suitable for analysis of geographical data. The flexibility in data formats and the possibility to import and export data in several data formats make the code easily compatible with other modelling tools used in the assessment.

3.4 CCSM4

3.4.1 Introduction

The American National Center for Atmospheric Research (NCAR) Community Climate System Model (CCSM) is a coupled atmosphere-ocean general circulation model for simulating the Earth's climate system. The CCSM is composed of four separate models simultaneously simulating the Earth's atmosphere, ocean, land surface and sea-ice, and one central coupler component, allowing researchers to conduct fundamental research into the Earth's past, present and future climate states (Gent et al. 2011).

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

Version 4 of CCSM ('CCSM4') was used in support of the SR-PSU (SKB TR-13-05) as a tool to evaluate the potential for cold climate conditions in the next 60 000 years (Brandefelt et al. 2013). The previous version of the code ('CCSM3') was used in support of the assessment of past and future climate in Forsmark (Kjellström et al. 2009) for the Spent nuclear fuel repository (see SKB TR-10-49). Both these studies are included as a basis for the post-closure safety assessment in the PSAR for SFR, see the **Climate report**, Sections 2.1.4 and 3.2.2.

The CCSM code is a category 3 code.

3.4.2 Documentation of the code

The CCSM4 users guide is found at www.cesm.ucar.edu/models/ccsm4.0/ccsm_doc/book1.html. The user's guide provides an overview of the components as well as instructions on acquiring the code and input data, running the code and post-processing the output data. Further, instructions for porting CCSM to a new machine as well as port validation is described in the user's guide.

The mathematical models and methods by which the solution is obtained for CCSM4, and the components of the coupled model, are described in detail at www.cesm.ucar.edu/models/ccsm4.0.

3.4.3 Development process and verification

The CCSM4 code was developed by the international climate research community over several decades. Gent et al. (2011) describe developments to all components in CCSM4, and document fully coupled pre-industrial control runs compared with runs with the previous version, CCSM3.

3.4.4 Rationales for using the code in the assessment

The CCSM4 code was selected for the post-closure safety assessment since it is one of the world-leaders in its field. Further, comparisons of the results for past, present and future projected climate, with other models in the field are available in scientific literature.

3.5 Comsol Multiphysics

3.5.1 Introduction

Comsol Multiphysics is a commercial finite element software for solving coupled partial differential equations. The code solves space and time dependent governing equations from a wide range of application areas, including fluid flow, heat transfer, mass transfer and chemical reactions, structural mechanics, and electromagnetics. In SR-PSU the code was primarily used to model the near-field hydrology (Abarca et al. 2013, 2014). It has also been used in the PSAR for an extension of the analysis performed in the SR-PSU (Abarca et al. 2020).

Comsol Multiphysics v4.3a (COMSOL 2012a) running under Windows has been used in the SRPSU assessment calculations. In the PSAR assessment calculations Comsol Multiphysics v5.3 (COMSOL 2017) has been used. The following add-on products have been used in addition to the base package:

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

The near-field hydrology models require input from the regional hydrogeology, pressure and flux boundary conditions as well as rock permeability fields that are calculated using the DarcyTools code. The modelling performed for the SR-PSU is also included as a basis for the PSAR.

Comsol Multiphysics including its modules is a widely used commercial code belonging to category 3.

3.5.2 Documentation of the code

Documentation of Comsol Multiphysics® version 5.3, used in this assessment and its modules, is provided by the code developer, Comsol AB (www.comsol.com). The developer provides technical support and software training, as well as an on-line forum for the Multiphysics modelling community. Comsol Multiphysics solves space and time dependent governing equations from a wide range of application areas, including fluid flow, heat transfer, mass transfer and chemical reactions, structural mechanics, and electromagnetics. The equations solved and the numerical methods used are described in the software documentation.

Material properties and physical data libraries are also provided by the developer or may be assigned directly as numerical values in the models. The interfaces to CAD software facilitate import of geometries. Existing models can readily be extended without restarting the modelling process or changing the simulation tool.

3.5.3 Development process and verification

Comsol Multiphysics is a widely used commercial code, supported by the QA processes of the code developer, Comsol AB.

3.5.4 Rationales for using the code in the assessment

Comsol Multiphysics is used in safety assessments for several reasons. One of the main benefits of the code is the ability to solve space and time dependent models of coupled processes in a flexible way. Furthermore, Comsol Multiphysics is a widely used commercial code, providing vendor QA, technical support, and documentation. The software offers interfaces to CAD software such that repository design geometries can be used directly in the technical analysis. Comsol Multiphysics also provides interfacing to technical computing software, and script programming in Java. This allows for user-defined extensions of the standard functionality as well as the opportunity to couple Comsol Multiphysics to other modelling tools used in the assessment.

3.6 DarcyTools

3.6.1 Introduction

DarcyTools is groundwater flow and transport modelling software developed collaboratively by SKB, CFE AB (Computer-aided Fluid Engineering AB) and MFRDC (Michel Ferry Research&Development Consulting), with SKB as the owner of the code. The code was developed to simulate flow and transport in porous and/or fractured media. It is a general code for this class of problems, but was developed for the analysis of fractured rock and porous media soil cover on top of the rock surrounding nuclear waste repositories.

Version 3.4 of the code was used to simulate groundwater flow in the SR-PSU (Odén et al. 2014). Version 4.0 of the code has been used in the PSAR for an extension of the analysis performed in the SR-PSU (Öhman and Odén 2018). The modelling performed for the SR-PSU is also included as a basis for the PSAR.

The code was previously used in the safety assessment for SR-Site (Forsmark and Laxemar), as described in Svensson and Follin (2010), Svensson and Rhén (2010) and Vidstrand et al. (2010a, b).

The code is regarded as a category 4b code as the user base is small and mainly limited to SKB projects.

3.6.2 Documentation of the code

The concepts, methods and equations used in DarcyTools version 3.4 are described in Svensson et al. (2010). This description is also valid for version 4.0.

The DarcyTools model uses human readable text files both as inputs and outputs.

Svensson and Ferry (2010) is a User's Guide that describes all the input parameters. These input parameters make up the CIF (Compact Input File), which is written in XML format. DarcyTools also includes a FORTRAN input file, where more advanced features (transient boundary conditions, new source/sink terms, etc) can be introduced.

Tecplot has been selected as the standard tool for post processing. Input files for Tecplot are readily generated.

An important aspect of the code is the ability to monitor the simulation on the computer screen. Convergence parameters, development of variables at control points or in profiles are plotted on the screen during the simulation. From v3.4 and onwards, it is even possible to plot the distribution of variables in specified planes.

3.6.3 Development process and verification

Development work on DarcyTools initiated in early 2001. The initial code built upon earlier groundwater models developed by CFE AB. The first well documented version of DarcyTools was v2.1, which was released in 2004. Versions 3.4 and 4.0 run under both Windows and Red Hat Linux.

Svensson (2010) describes the verification, validation and demonstration of version 3.4 of DarcyTools. About thirty simple test cases, most with an analytical solution, are used to ensure that the equations are solved correctly. When a new major version of the code is released, all test cases are updated and checked to ensure both consistency with the old version and to make sure that the new version is correct. Validation is considered to be the process by which the code is shown to agree with measured data ("the right equations are solved"). Therefore, a number of comparisons with field data are included. So far, no attempt has been made to show that DarcyTools conforms to any international QA standard.

3.6.4 Rationales for using the code in the assessment

DarcyTools has been selected for use in the safety assessment because it is a code developed in cooperation with SKB especially for solving flow-related problems within nuclear waste management. The addition of efficient tailor-made features makes DarcyTools a suitable code for a wide range of problems that need to be considered by SKB.

3.7 Ecolego

3.7.1 Introduction

Ecolego is a flexible software tool for modelling dynamic systems (systems of ordinary differential equations) and performing deterministic or probabilistic simulations. 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 commercial software and is used by companies and institutions all over the world.

Ecolego is used as a tool for modelling and performing simulations of radionuclide transport and dose to humans as well as dose rates to non-human biota (NHB) in SKB´s post-closure safety assessments. In the SR-PSU Ecolego was used for modelling and performing simulations of radionuclide transport in the nearfield, geosphere and biosphere. The modelling performed for the SR-PSU is included as a basis for the PSAR.

Ecolego was also used in the SR-Site safety assessment to perform supporting radionuclide transport and dose calculations in the surface systems (SKB TR-10-09) as well as in the evaluation of post-closure safety for a proposed repository concept for SFL (SKB TR-19-01).

The version of the code used in the SR-PSU was Ecolego 6.0. In the PSAR version 6.5 for both Windows 10 Enterprise (64 bit) and Linux is used.

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

3.7.2 Documentation of the code

Ecolego has a comprehensive homepage (https://ecolego.se) and web-based user guide (https://resources.facilia.se/ecolegowiki/doku.php) which is continuously updated by the developer. The user guide provides guidance for the use of the code, with step by step tutorials for the novice user and also full description of all implemented methods and features. At the same web site, there is also access to other resources such as a forum for support, ideas, answers and community talk as well as an issue tracker to report bugs and request improvements. For Ecolego 6 or previous versions, information is available at http://old.ecolego.facilia.se.

Ecolego has been designed to maximise transparency and flexibility, while at the same time offering 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.

The correct usage of the code in the SR-PSU safety assessment, is assured as Ecolego was used in close collaboration with the developer of the code.

The mathematical models implemented in Ecolego for the PSAR safety assessment are described in detail in Åstrand et al. (2022) and in Saetre et al. (2013).

3.7.3 Development process and verification

Ecolego is widely used commercial software, supported by the QA processes of the code developer, AFRY AB (the code was acquired by AFRY in 2018).

Ecolego has been developed since 2002 and has been verified and validated through several comparisons with both analytical solutions and with benchmarks of other software such as Amber and Simulink (Maul et al. 2004).

3.7.4 Rationales for using the code in the assessment

Ecolego is used in the safety assessment because the code is very suitable for probabilistic risk assessments of complex dynamic systems evolving over time with a large number of species. Ecolego has databases and other add-ons especially designed for the field of radiological risk assessment. The code is well known by SKB employees and consultants, many of whom have been involved in the development of the code.

3.8 FASTREACT

3.8.1 Introduction

FASTREACT was developed by SKB to perform quick probabilistic reactive transport calculations (Trinchero et al. 2014c).

FASTREACT has been used in the SR-PSU in the modelling of the geochemical evolution in the geosphere (Román-Ross et al. 2014). The modelling performed for the SR-PSU is also included as a basis for the PSAR.

FASTREACT was also used to model the hydrogeochemical evolution for the Finnish safety case TURVA2012 (Trinchero et al. 2014b).

FASTREACTS belongs to category 4b.

FASTREACT is based on the theory of Stochastic-Convective (SC) models (Shapiro and Cvetkovic 1988). In this context, the breakthrough curve of the tracer, $\overline{C}(t)$, can be described as a simple temporal convolution of the inflow concentration $c_{in}(t)$, and the probability distribution function (PDF) of solute travel times along the considered set of independent streamlines, $p(t)$.

This travel time PDF, also denoted as a transfer function, can be used to get insight into key features of the medium such as its textural structure and heterogeneity in hydraulic properties, including the degree of preferential flow.

The intrinsic efficiency of stochastic-convective models makes them particularly suitable for the solution of reactive transport problems. For these applications, solving a set of one-dimensional problems is in most cases computationally much less expensive than solving for transport in a single multidimensional system.

FASTREACT is suited for post-closure safety assessment calculations as the travel time PDF is directly derived from particle tracking calculations run using a related hydrogeological model (DarcyTools in the case of the SR-PSU and the PSAR).

3.8.2 Documentation of the code

Comprehensive documentation of the code and methodology can be found in Trinchero et al. (2014c).

3.8.3 Development process and verification

FASTREACT was developed using a test-driven development cycle. New validation tests were added when new functionality was developed or when bugs were found in uncovered portions of code. Verification tests are included in Trinchero et al. (2014c). FASTREACT was validated against independent solutions in different benchmark cases (Trinchero et al. 2014a, c).

FASTREACT runs in Python 3. All input data and output results are handled by using Python scripts. This allows for a full traceability of the process.

3.8.4 Rationales for using the code in the assessment

The rationale for selecting FASTREACT in the post-closure safety assessment was its high efficiency and the fact that results are consistent with transport pathways (i.e. distribution of travel times) computed from hydrogeological models.

3.9 LOVECLIM

3.9.1 Introduction

The LOVECLIM is a coupled Earth system model of intermediate complexity. It includes the dynamics of the atmosphere, ocean and sea-ice and vegetation (Goosse et al. 2010).

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

Version 1.2 of LOVECLIM was used in support of the assessment of future climate in Forsmark in the SR-PSU (SKB TR-13-05) as a tool to evaluate the potential for cold climate conditions in the next 60 000 years (Brandefelt et al. 2013). This study is included as a basis for the post-closure safety assessment in the PSAR for SFR, see the **Climate report**, Section 2.1.4.

The LOVECLIM code is a category 3 code.

3.9.2 Documentation of the code

Documentation on usage of LOVECLIM is found at https://www.elic.ucl.ac.be/modx/index.php?id=81. The mathematical models and methods by which the solution is obtained for the LOVECLIM, and the components of the coupled model, are described in Goosse et al. (2010).

3.9.3 Development process and verification

The first two components of LOVECLIM, which were coupled at the end of the 1990s, were the atmospheric model ECBilt and the sea–ice–ocean model CLIO, forming ECBilt-CLIO2. These two components are still the core of LOVECLIM, but have been improved significantly compared with the original versions, see Goosse et al. (2010).

3.9.4 Rationales for using the code in the assessment

The code was selected for the post-closure safety assessment since it is considered well suited for the longer timescales considered and one of the world-leaders in its field.

3.10 MIKE SHE

3.10.1 Introduction

The near-surface hydrological and hydrogeological code MIKE SHE (Système Hydrologique Européen) is a commercial code developed by the Danish Hydraulic Institute (DHI). The code describes the main processes in the land phase of the hydrological cycle, from rainfall to river flow (Graham and Butts 2005). Transport calculations, particle tracking and advection–dispersion calculations can also be performed within the MIKE SHE modelling tool.

MIKE SHE Version 2012 (DHI 2012) was used in the SR-PSU to model the hydrology and near-surface hydrogeology for present and future conditions and under different climate conditions (Werner et al. 2013, **Biosphere synthesis report**). An extension of the SR-PSU work performed for the PSAR (**Biosphere synthesis report**). The modelling performed for the SR-PSU is also included as a basis for the PSAR. MIKE SHE version 2009 was used in the SR-Site safety assessment. The main difference between version 2012 and 2009 is the possibility to work with time varying properties.

The system is certified for Windows XP Professional Service Pack 3 (32 bit), Windows Vista Business Service Pack 2 (64 bit) and Windows 7 Professional Service Pack 1 (32 and 64 bit). In the SR-PSU modelling both the Windows XP and Windows 7 systems have been used.

The MIKE SHE model is a category 3 code.

3.10.2 Documentation of the code

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

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

3.10.3 Development process and verification

The MIKE SHE software originates from the Système Hydrologique Européen (SHE) model, which became operational in 1982. The model was developed by three organisations; the British Institute of Hydrology, the French consulting company SOGREAH and the Danish Hydraulic Institute, DHI, which markets the MIKE SHE software today (http://www.mikepoweredbydhi.com/).

There is a direct coupling between MIKE SHE and the GIS program ArcMap which is part of the ArcGIS framework, see Section 3.3. This is advantageous, because 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 performed in the ArcGIS program (see Section 3.3). This ensures an acceptable level of quality as well as a high level of traceability for the input data to the model.

An ASCII log-file is produced for each simulation. This file can be used to check for errors, warnings and issues such as convergence. The MIKE SHE model can also be run using a Graphical User Interface (GUI), which is documented in an on-line User Manual.

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

3.10.4 Rationales for using the code in the assessment

MIKE SHE is a well-established tool for hydrology and near surface hydrogeology calculations. MIKE SHE makes it possible to model the interactions between surface water, groundwater and evaporation processes and makes it possible to describe and understand the complexity of water flow in the surface system of importance for transport in the biosphere.

3.11 Numerical GIA model

3.11.1 Introduction

The GIA (Glacial Isostatic Adjustment) code is designed to calculate the isostatic adjustment of the solid earth due to loading and unloading of ice and water during a glacial cycle. The code was developed at the University of Toronto.

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

The GIA code was used to determine relative sea-level and shoreline positions at Forsmark for the reconstruction of the last glacial cycle and for a warmer future climate development for SR-Site (Section 3.3.4 in SKB TR-10-49). The results of that study are judged to be adequate for assessment purposes and are thus used also for the SR-PSU and the PSAR SFR (**Climate report**).

The GIA code is a category 4b code since the user base is small.

3.11.2 Documentation of the code

The GIA code is written in FORTRAN, and has been developed by Dr. G.A. Milne and Prof. J.X. Mitrovica at the University of Toronto (Milne 1998, Milne and Mitrovica 1998, Milne et al. 1999). The code is used by a small user base of postgraduate students and postdoctoral researchers working in either Milne's or Mitrovica's research groups. Due to the nature of the development of the GIA code, and the intended user base, there is no formal documentation available. The version of the code used to determine relative sea-level and shoreline positions at Forsmark, run on UNIX computing platform at the university of Durham, and is the one described in Mitrovica and Milne (2003). Correct use was assured by working in close collaboration with the developer of the code.

3.11.3 Development process and verification

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 over the years to account for several different processes, and thus, to improve the accuracy of the computation. The theory that the version of the code used for the safety assessments is based on and the algorithm employed to solve the governing equations are described in Mitrovica and Milne (2003), Kendall et al. (2005) and Latychev et al. (2005).

In the code development, the accuracy of the numerical schemes employed was tested through comparison with several analytical solutions. The code has several built-in analytical checks to ensure that the output is correct.

A small number of research groups have developed their own sea-level codes based on the results presented in the papers referenced above. The solid earth response to GIA-loading has been successfully benchmarked between several groups, summarised in Spada et al. (2011) (https://doi.org/10.1111/j.1365-246X.2011.04952.x).

3.11.4 Rationales for using the code in the assessment

The code was selected for the post-closure safety assessment because it is one of the world-leaders in its field.

3.12 Numerical permafrost model

3.12.1 Introduction

The numerical permafrost model code, is designed to calculate the development of permafrost and perennially frozen ground.

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 TR-06-23).

The third version of the code was used in the SR-PSU to investigate the potential for permafrost in the next 60 000 years in Forsmark (**Climate report**). Results of a study of permafrost and perennially frozen ground in a 2D vertical cross-section at Forsmark (Hartikainen et al. 2010) performed for SR-Site were also used in the SR-PSU. That study was performed with the second version of the code. Both studies are also used in support of the PSAR.

The code is classified as a category 4b code since it was developed for post-closure safety assessments and is only used by a small group of users.

3.12.2 Documentation of the code

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

3.12.3 Development process and verification

The numerical permafrost model code, written in FORTRAN, was originally developed at Helsinki University of Technology for soil freezing problems (Hartikainen 1994) being built on a general finite element solver code for non-linear non-stationary problems (Freund and Lempinen 1994). The first version of the permafrost model code was written for the international project DECOVALEX III to investigate thermo-hydro-mechanical impacts of processes associated with freezing and thawing of the subsurface during periods of glaciation/deglaciation on the post-closure safety of a hypothetical repository (Hartikainen 2004, Chan et al. 2005). Thereafter, the second version of the code was developed for post-closure safety assessments to represent a 2D vertical cross-section (Hartikainen et al. 2010). This version deals with spatially varying surface conditions and salt transport as well as addressing the solution of large systems of equations. The code was further updated for the SR-PSU to include seasonal freezing and thawing of the ground (Brandefelt et al. 2013).

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, ii) the effects of pressure and salinity on the temperature of the groundwater, and (iii) salt freezing and salt transport in partially frozen soil.

The validation of the density-controlled groundwater flow showed that the model gave a slightly faster development of the salt concentration as compared with a benchmark test. The validation further showed good agreement with experimental observations of gravity driven convection of salt. Validation of the effects of pressure and salinity on the freezing temperature showed that the model generates data in very good agreement with experimental reference data. The validation of salt freezing also showed that the model produces data in accordance with large-scale laboratory tests. All in all, these benchmark and laboratory model evaluations, including the one on density-controlled groundwater flow, show that the model is suitable to use for the purposes of the safety assessment.

The model development and verification of the third version of the code as well as the consistency of results between the third and second version of the code can be found in Brandefelt et al. (2013). The validations described above, 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 safety assessment.

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 the temperature of 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 conditions, 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 (vertical bedrock temperature distribution at the GAP-04 drillsite (Claesson Liljedahl et al. 2016)) comes from the GAP project, see further SKB's research, development and demonstration (RD&D) programme (SKB 2022).

3.12.4 Rationales for using the code in the assessment

The code was selected for the safety assessment since it is one of the world-leaders in its field.

3.13 PHAST

3.13.1 Introduction

PHAST (Parkhurst et al. 2004, 2010) simulates multi-component, reactive transport in saturated 1, 2 or 3D groundwater flow systems. PHAST is a versatile groundwater flow and solute transport simulator with the capability to model a wide range of equilibrium and kinetic geochemical reactions. The flow and the transport calculations use a modified version of HST3D (Kipp 1987, 1997) that is restricted to constant fluid density and constant temperature. The geochemical reactions are simulated with PHREEQC (Parkhurst and Appelo 1999, 2013), which is embedded in PHAST.

PHAST was used in the SR-PSU for investigating the impact of fractures on the rate of concrete degradation in the barriers (Höglund 2014). The modelling performed for the SR-PSU is also included as a basis for the PSAR. In the PSAR assessment calculations PHAST has been used to predict pH evolution (Höglund 2019).

PHAST has also been used as a numerical tool in a number of previous safety assessment studies for SKB (Arcos et al. 2006, Grandia et al. 2006, 2007, Luna et al. 2006, Domènech et al. 2006, Sena et al. 2008, 2010).

Because the code is open source, with a large user base and was not written exclusively nor modified for SKB projects, it is regarded as a category 3 code.

3.13.2 Documentation of the code

PHAST is explained in detail and example calculations are provided in the user's manual (Parkhurst et al. 2004, 2010). In addition to this, information, well documented examples and an active and interactive FAQ section are provided on USGS web site https://www.usgs.gov/software/phast-computer-program-simulating-groundwater-flow-solute-transport-and-multicomponent.

Data files are built with modular keyword data blocks and the spatial data are defined in 3D rectangular zones. All this information is easily introduced by means of .dat files.

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

3.13.3 Development process and verification

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

The code is regularly updated, and both the code and its revision history are available at https://water.usgs.gov/water-resources/software/PHAST/.

3.13.4 Rationale for using the code in the assessment

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

3.14 PHREEQC

3.14.1 Introduction

PHREEQC (pH-REdox-EQuilibrium-C) is a computer program written in the C programming language, and is a robust geochemical code designed to perform a wide variety of low-temperature aqueous geochemical calculations.

PHREEQC can be used to perform speciation and saturation-index calculations, and batch-reaction and one-dimensional (1D) transport calculations (dispersion, diffusion and various other parameters to be defined for dual porosity media). The code may be used to calculate the interaction of aqueous solutions with minerals, gases, solid solutions, ion exchangers and sorption surfaces. It also has the capability to include kinetic reactions with user-defined rate expressions.

PHREEQC has been used in SKB's post-closure safety assessments, Project SAFE, SR-Can, SR-Site, and SAR-08, and elsewhere, see Höglund (2001), Duro et al. (2006), Grivé et al. (2010) and Guimerà et al. (2006).

The modelling performed for the SR-PSU in PHREEQC is included as a basis for the PSAR. In the SR-PSU, PHREEQC version 2 was used for predicting and constraining redox conditions (Auqué et al. 2013, Gimeno et al. 2008, Gimeno et al. 2011, Duro et al. 2012) and the temporal variability in pH (Cronstrand 2014, Höglund 2014) in the repository and groundwater, and to approximate cement pore water compositions or groundwater interactions with cement material in general (Crawford 2013, Cronstrand 2014, Höglund 2014).

For the PSAR, PHREEQC version 3 has been used to calculate the evolution of pH in the 1BRT and the 2BMA compartments in the SFR repository (Höglund 2018, 2019), and to estimate the speciation and solubility of various radionuclides in the presence of complexing agents (Bruno et al. 2017, Keith-Roach and Shahkarami 2021).

The PHREEQC code is an opensource code with a large user base and is here regarded as a category 3 code.

Noteworthy here is that PHREEQC requires thermodynamic data (reaction stoichiometry, equilibrium constants, etc) stored in thermodynamic databases for equilibrium calculations, with some default thermodynamic databases supplied together with the code. The default thermodynamic databases may be modified according to user needs, alternatively externally compiled thermodynamic databases may be used. The thermodynamic data stored in the thermodynamic databases are hence regarded as input data to the model rather than a functionality of the code itself.

3.14.2 Documentation of the code

The PHREEQC version 2 user's manual (Parkhurst and Appelo 1999) describes the program in detail (https://pubs.er.usgs.gov/publication/wri994259) and examples on the geochemical and transport equations that can be solved using this code are provided. The web pages of both authors (https://www.hydrochemistry.eu/ and https://www.usgs.gov/software/phreeqc-version-3) also contain information, well documented examples, and an active and interactive frequently asked questions (FAQ) section.

PHREEQC version 3 extends PHREEQC version 2 with several features. These additions are all explained in detail in the PHREEQC version 3 user's manual (Parkhurst and Appelo 2013) (https://pubs.er.usgs.gov/publication/tm6A43).

3.14.3 Development process and verification

PHREEQC is an opensource code developed by the United States Geological Survey. Updated versions are released regularly. The code and revision history are available on https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/.

PHREEQC is widely used and its algorithm has been checked in several scientific publications and through the example files distributed with the computer program.

3.14.4 Rationales for using the code in the assessment

The PHREEQC code has been used in the safety assessment to perform speciation calculations using thermodynamic equilibrium data. PHREEQC is widely used and well supported for this purpose.

3.15 UMISM

3.15.1 Introduction

UMISM (University of Maine Ice Sheet Model) is a 3D thermo-mechanical ice-sheet model designed to simulate realistic ice sheets.

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 TR-06-23, SKB R-08-130, SKB TR-10-49).

UMISM was used in support of SR-Site to reconstruct the ice sheet of the last glacial cycle, to construct a reference glacial cycle, and as input to simulations of other phenomena such as permafrost, isostatic changes, crustal stress, and ground water flow. The ice sheet model results obtained within SR-Site for the Forsmark site (SKB TR-10-49) were judged as adequate to use as a basis also for the SR-PSU and the PSAR (**Climate report**).

The code is classified as a category 4b code.

3.15.2 Documentation of the code

Due to the nature of the development of the UMISM code, and the intended user base, there is no formal documentation available. Descriptions of model setups, and simulations are found in the **Climate report**, Section 2.3.4. The close collaboration with the developer of the code assures the correct usage of the code.

3.15.3 Development process and verification

The UMISM finite-element code, written in FORTRAN, was originally developed by Prof. J. Fastook, at the School of Computing and Information Science at University of Maine, U.S.A., (e.g. Fastook and Chapman 1989, Fastook 1990, 1994, Fastook and Holmlund 1994, Fastook and Prentice 1994, Johnson 1994). The version of UMISM as of October 2004/April 2005 was used for the study performed for SR-Site.

As discussed in the **Climate report**, Section 2.3.4, 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 agree well with these other models (Huybrechts et al. 1996, Payne et al. 2000). The model uncertainties are reported in the **Climate report**, Section 2.3.7.

UMISM was compared with, and shown to be capable of producing an account of the general development of the Weichselian ice sheet which complies with the overall Weichselian glacial history as known from Quaternary geology, glacial morphology, etc studies (**Climate report**, Sections 2.3.4 and 3.2).

In addition, UMISM was compared and shown to provide similar results as completely different types of ice sheet models (ICE-5G (Peltier 2004) and ANU (Lambeck et al. 2010) that 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.

3.15.4 Rationales for using the code in the assessment

The UMISM code was selected for the safety assessment because several simulations of the Fennoscandian ice sheet have been carried out with the UMISM model over the years. This has resulted in considerable experience and understanding of how to perform model calibrations against geological observations in order to obtain more realistic ice sheet configurations.

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Appendix A

Terms and abbreviations

Terms and abbreviations used in this report are explained in Table A-1.

Table A-1. Explanations of terms and abbreviations used in this report.

Name	Description
1–2BMA	Vaults for intermediate-level waste in SFR.
1–2BTF	Vaults for concrete tanks in SFR1.
1–5BLA	Vaults for low-level waste in SFR.
1BLA	Vault for low-level waste in SFR1.
1BMA	Vault for intermediate-level waste in SFR1.
1BRT	Vault for reactor pressure vessels in SFR3.
1D	One-dimensional.
2–5BLA	Vaults for low-level waste in SFR3.
2BMA	Vault for intermediate-level waste in SFR3.
2BTF	Vault for concrete tanks in SFR1.
2D	Two-dimensional.
3D	Three-dimensional.
3DEC	Computer code used for modelling rock stability over time.
5BLA	Vault for low-level waste in SFR3.
AD	Anno Domini.
ADINA	A computer code used to calculate stresses due to an earthquake.
AMBER	Assisted Model Building with Energy Refinement, a compartmental computer code.
AMF	Assessment model flowchart.
AP	After Present.
Assessment team	The group of persons responsible for performing the safety assessment. The team judge the material delivered by the data supplier and recommend data for use in the assessment.
Barrier	In the safety assessment context, a barrier is a physical feature, engineered or natural, which in one or several ways contributes to the containment and retention or prevention of dispersion of radioactive substances, either directly or indirectly by protecting other barriers.
Bedrock	In the safety assessment context, the solid rock beneath the regolith also including the groundwater in the rock.
BLA	Vault for low-level waste.
BMA	Vault for intermediate-level waste.
BTF	Vault for concrete tanks.
CCSM	Community Climate System Model, a coupled model for simulating the Earth's climate system.
CMIP	Coupled Model Intercomparison Project, a collaborative framework designed to improve knowledge about climate change.
COMSOL Multiphysics	Commercial software for finite element analysis, solver and multi-physics simulation software.
DarcyTools	A computer code developed by SKB for simulation of flow and transport in porous and/or fractured media.
DEM	Digital elevation model. Describes the topography and bathymetry of the modelled area.
Exposure	The act or condition of being subject to irradiation (not to be used as a synonym for dose, which is a measure of the effects of exposure).
FASTREACT	Computer code for reactive transport simulations along a set of streamlines based on mechanistic and geochemical processes.
GAP	The Greenland Analogue Project, a multilateral research project on the west coast of Greenland.
Geosphere	The bedrock, including groundwater, surrounding the repository, bounded above by the surface system.
GIA	Glacial isostatic adjustment.
GIS	Geographical information system.

Table A-1. Continued.

Name	Description
ICE-5G	A global ice sheet reconstruction.
Initial state	The expected state of the repository and its environs at closure of the repository.
Intermediate-level waste	Radioactive waste that requires final disposal in a geological repository and shielding during handling. Cooling of the waste is not required.
IPCC	Intergovernmental Panel on Climate Change.
KBS-3	Method developed by SKB for final disposal of spent nuclear fuel.
Long-lived radionuclide	In the safety assessment context, radionuclides with a half-life exceeding 31 years.
LOVECLIM	LOch–Vecode-Ecbilt-CLio-agIsm Model (Climate model of intermediate complexity).
Low-level waste	Radioactive waste that requires final disposal in a geological repository. Shielding during handling and cooling are not required.
Mathematical model	A quantitative description of a physical system, where important processes and components, and interactions between components, are represented by parameters and equations.
MIKE SHE	Computer code used to simulate groundwater and surface water flow.
NCAR	National Center for Atmospheric Research (USA).
Near-field	Typically used for the model domain representing the repository, which may contain part of the nearby bedrock to obtain boundary conditions.
NHB	Non-human biota.
NRPA	Norwegian Radiation Protection Authority
Packaging	The outer container, such as a mould, drum or ISO-container, protecting the waste form (synonymous with Waste packaging).
PDF	Probability density function.
PHAST	Computer code used, for example, for concrete degradation calculations and geochemical evolution in the geosphere.
PHREEQC	Computer code used for geochemical modelling of the evolution of repository pH and redox.
Protective capability	The capability to protect human health and the environment from the harmful effects of ionising radiation.
PSAR	Preliminary Safety Analysis Report.
PSAR SFR	Preliminary Safety Analysis Report for the extended SFR.
PSU	Programme SFR extension.
QA	Quality assurance.
RDC	Reducing capacity.
Reference evolution	The probable post-closure evolution of the repository and its environs, including uncertainties in the evolution that may affect the protective capability of the repository.
Regolith	All matter overlying the bedrock. This includes both minerogenic and organogenic (i.e. derived from organic substances) deposits.
Repository	The disposed waste packages, the engineered barriers and other repository structures.
Risk	Refers in the post-closure safety assessment to the radiological risk, defined as the product of the probability of receiving a radiation dose and the harmful effects of that radiation dose.
SAFE	Post-closure safety assessment for SFR1 reported to the regulatory authorities in 2001.
Safety analysis	In the context of the present safety assessment, the distinction is generally not viewed as important and therefore safety analysis and safety assessment are used interchangeably. However, if the distinction is important, safety analysis should be used as a documented process for the study of safety and safety assessment should be used as a documented process for the evaluation of safety.
Safety assessment	The safety assessment is the systematic process periodically carried out throughout the lifetime of the repository to ensure that all the relevant safety requirements are met and entails evaluating the performance of the repository system and quantifying its potential radiological impact on human health and the environment. The safety assessment corresponds to the term safety analysis in the Swedish Radiation Safety Authority's regulations.
SAR	Safety Analysis Report.
Scenario	A description of a potential evolution of the repository and its environs, given an initial state and specified external conditions and their development and how the protective capability of the repository is affected.
SFL	Final repository for long-lived radioactive waste.
SFR	Final repository for short-lived radioactive waste at Forsmark.
SFR1	The existing part of SFR.
SFR3	The extension part of SFR.

Table A-1. Continued.

Name	Description
Shoreline displacement	The movement of the shoreline, that is the variation in time of the spatial location of the shoreline.
Silo	Cylindrical vault for intermediate-level waste (part of SFR1).
SKB	Swedish Nuclear Fuel and Waste Management Company.
SR-Can	Preliminary post-closure safety assessment for the planned spent nuclear fuel repository, published in 2006.
SR-PSU	Post-closure safety assessment that was a reference to the F-PSAR for the extended SFR, reported to the regulatory authority in 2014.
SR-Site	Post-closure safety assessment for a spent nuclear fuel repository in Forsmark, reported to the regulatory authority in 2011.
SSM	Swedish Radiation Safety Authority.
Surface system	In the safety assessment context, refers to the part of the repository system that is above the geosphere, with all its abiotic and biotic processes and features, as well as humans and human behaviour. Synonymous with Biosphere system.
UMISM	University of Maine Ice Sheet Model.
Waste form	Waste in its physical and chemical form after treatment and/or conditioning.
Waste vault	Part of repository where waste is disposed.

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SKB is responsible for managing spent nuclear fuel and radioactive waste produced by the Swedish nuclear power plants such that man and the environment are protected in the near and distant future.

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