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Technical Report 14-09

Provisional Safety Analyses for SGT Stage 2

Models, Codes and General Modelling Approach

Dezember 2014

National Cooperative
for the Disposal of
Radioactive Waste

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The report was fully reviewed by Peter Robinson, David Lever and Jürg W. Schneider. Additional comments were provided by Russell Walke, Jens K. Becker and Veerle Cloet. The authors would like to thank the reviewers for their valuable contributions.

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Summary

In the framework of the provisional safety analyses for Stage 2 of the Sectoral Plan for Deep Geological Repositories (SGT), deterministic modelling of radionuclide release from the barrier system along the groundwater pathway during the post-closure period of a deep geological repository is carried out. The calculated radionuclide release rates are interpreted as annual effective dose for an individual and assessed against the regulatory protection criterion 1 of 0.1 mSv per year. These steps are referred to as dose calculations. Furthermore, from the results of the dose calculations so-called characteristic dose intervals are determined, which provide input to the safety-related comparison of the geological siting regions in SGT Stage 2. Finally, the results of the dose calculations are also used to illustrate and to evaluate the post-closure performance of the barrier systems under consideration.

The principal objective of this report is to describe comprehensively the technical aspects of the dose calculations. These aspects comprise:

- the generic conceptual models of radionuclide release from the solid waste forms, of radionuclide transport through the system of engineered and geological barriers, of radionuclide transfer in the biosphere, as well as of the potential radiation exposure of the population,
- the mathematical models for the explicitly considered release and transport processes, as well as for the radiation exposure pathways that are included,
- the implementation of the mathematical models in numerical codes, including an overview of these codes and the most relevant verification steps,
- the general modelling approach when using the codes, in particular the generic assumptions needed to model the near field and the geosphere, along with some numerical details,
- a description of the work flow related to the execution of the calculations and of the software tools that are used to facilitate the modelling process, and
- an overview of the quality assurance measures carried out.

Site-specific information used in the dose calculations is not documented in this report. Rather, it is compiled in Nagra (2014b) with links to other reports. The report Nagra (2014b) further describes the set of processes and parameters that are relevant to the provisional safety analyses, the definition of the calculation cases for the dose calculations and a discussion of the results. In this way, the report Nagra (2014b) and the present report together provide the required transparency and traceability with respect to the dose calculations for SGT Stage 2.

Other models and codes (e.g. groundwater models, mechanistic sorption models) that are used for the derivation of input parameters and for the justification of assumptions and simplifications used in this report are not described, but are dealt with in specific reference reports. The present report only occasionally refers to other reference reports; a more comprehensive presentation of the scientific basis for the dose calculations is given in Nagra (2014b).

Zusammenfassung

Im Rahmen der provisorischen Sicherheitsanalysen für Etappe 2 des Sachplans geologische Tiefenlager (SGT) werden deterministische Modellrechnungen zur Radionuklidfreisetzung aus dem System der technischen und geologischen Barrieren über den Grundwasserpfad für den Zeitraum nach Verschluss eines geologischen Tiefenlagers durchgeführt. Die berechneten Freisetzungsraten werden in eine jährliche effektive Individualdosis umgerechnet und dem behördlichen Schutzkriterium 1 von 0.1 mSv/a gegenübergestellt. Beide Schritte werden zusammenfassend als Dosisberechnungen bezeichnet. Aus den Ergebnissen der Dosisberechnungen werden ausserdem sogenannte charakteristische Dosisintervalle bestimmt, welche in den sicherheitstechnischen Vergleich der geologischen Standortgebiete in SGT Etappe 2 einfliessen. Schliesslich werden die Ergebnisse der Dosisberechnungen auch für die Illustration und die Bewertung der Wirksamkeit der untersuchten Barrierensysteme verwendet.

Ziel dieses Berichts ist die Bereitstellung der modelltechnischen Grundlagen für die Durchführung der Dosisberechnungen. Diese umfassen:

- die generischen konzeptuellen Modelle zur Mobilisierung der Radionuklide aus den festen Abfallbestandteilen, zum Radionuklidtransport durch das System der technischen und geologischen Barrieren, zum Verhalten der Radionuklide in der Biosphäre sowie zur resultierenden potentiellen Strahlenexposition für die Bevölkerung,
- die mathematischen Modelle zur Beschreibung der explizit berücksichtigten Freisetzungs- und Transportprozesse, sowie der einbezogenen Strahlenexpositionspfade,
- die Umsetzung der mathematischen Modelle in numerischen Rechencodes, inklusive einer zusammenfassenden Beschreibung dieser Codes sowie der wichtigsten Verifizierungsschritte,
- das allgemeine Vorgehen bei der Anwendung der Rechencodes auf die untersuchten Barrierensysteme, im Speziellen die generischen Annahmen zur Modellierung des Nahfelds und der Geosphäre, sowie numerische Aspekte,
- eine Beschreibung der Arbeitsabläufe bei der Durchführung der Modellrechnungen und der verwendeten Werkzeuge zur Organisation der Modellierungsarbeiten, sowie
- eine Übersicht zu den durchgeführten Qualitätssicherungsmassnahmen.

Standortspezifische Grundlagen für die Dosisberechnungen sind nicht Teil dieses Berichts. Diese sind in Nagra (2014b) mit Verweis auf weitere Berichte zusammengestellt. Der Bericht Nagra (2014b) enthält auch eine Zusammenstellung der für die provisorischen Sicherheitsanalysen relevanten Prozesse und Parameter, die Ableitung der Rechenfälle für die Dosisberechnungen sowie eine Diskussion der Resultate. Somit gewährleisten der Bericht Nagra (2014b) und der vorliegende Bericht zusammen die Transparenz und Nachvollziehbarkeit der Dosisberechnungen für SGT Etappe 2.

Andere Modelle und Rechencodes (z.B. Grundwassermodelle, mechanistische Sorptionsmodelle), welche für die Herleitung von Parameterwerten und für die Begründung von Modellannahmen und Vereinfachungen im Rahmen der vorliegenden Dosisberechnungen herangezogen werden, sind ebenfalls nicht Teil dieses Berichts, sondern werden in den jeweiligen Referenzberichten behandelt. Dieser Bericht verweist nur vereinzelt auf andere Referenzberichte, eine umfassendere Darstellung der wissenschaftlichen Grundlagen für die Dosisberechnungen ist in Nagra (2014b) enthalten.

Résumé

Dans le cadre des analyses de sûreté provisoires requises à l'étape 2 du plan sectoriel « Dépôts en couches géologiques profondes » (ci-dessous : « plan sectoriel »), on effectue des modélisations déterministes relatives au relâchement des radionucléides hors du système de barrières techniques et géologiques par le biais des eaux souterraines au cours de la phase de post-fermeture du stockage géologique. Les taux de relâchement calculés sont exprimés en termes de dose efficace individuelle annuelle, que l'on compare au critère de protection n°1 de l'autorité de sûreté, à savoir 0.1 mSv/a. On utilise le terme « calculs de dose » pour désigner ces deux étapes de calcul. A partir des résultats des calculs de dose, on détermine en outre des « intervalles de doses caractéristiques », qui sont utilisés pour la comparaison des régions d'implantation géologiques du point de vue de la sûreté, telle qu'elle est prévue à l'étape 2 du plan sectoriel. Les résultats des calculs de dose servent également à illustrer et évaluer l'efficacité post-fermeture des systèmes de barrières de confinement envisagés.

L'objectif du présent rapport est de présenter de manière détaillée les bases techniques sur lesquelles reposent les calculs de dose, à savoir:

- les modèles conceptuels génériques relatifs à la mobilisation des radionucléides issus des déchets solides, au transport des radionucléides au travers du système de barrières techniques et géologiques, au comportement des radionucléides dans la biosphère et à l'exposition potentielle qui en résulte pour la population,
- les modèles mathématiques utilisés pour décrire les processus de relâchement et de transport des radionucléides qui ont été explicitement pris en compte, ainsi que les modes d'exposition considérés,
- la conversion des modèles mathématiques en modèles numériques, complétée par un aperçu des codes de calcul et des principales étapes de vérification,
- l'approche générale qui gouverne la mise en œuvre des codes de calcul, en particulier les hypothèses génériques et certains aspects numériques relatifs à la modélisation du champ proche et de la géosphère,
- une description de la procédure adoptée pour effectuer les calculs et une présentation des outils informatiques utilisés pour gérer les travaux de modélisation, ainsi que
- une liste des mesures d'assurance qualité mises en œuvre.

Le présent rapport ne comporte pas de données relatives à des sites spécifiques. Ces informations figurent dans le rapport Nagra (2014b), qui lui-même renvoie à d'autres rapports. Le rapport Nagra (2014b) décrit en outre les processus et paramètres pris en compte dans les analyses provisoires de sûreté, présente les cas de calcul pour lesquels les calculs de dose ont été effectués, et enfin présente les résultats obtenus. De cette façon, le rapport Nagra (2014b) et le présent rapport se complètent mutuellement pour répondre aux exigences de transparence et de traçabilité relatives aux calculs de dose pour l'étape 2 du plan sectoriel.

Ce rapport ne détaille pas non plus les autres modèles et codes de calculs utilisés pour déterminer les valeurs de paramètres et justifier les hypothèses de modélisation et de simplification dans le cadre des calculs de dose présentés (p. ex. les modèles relatifs aux écoulements d'eau souterrains ou les modèles mécanistes de sorption). Ces modèles et codes de calcul font l'objet de rapports de référence séparés. Le présent rapport ne renvoie à d'autres rapports de référence que dans des cas isolés. Pour une présentation plus complète de l'ensemble des bases scientifiques qui sous-tendent les calculs de dose, le lecteur est prié de consulter le rapport Nagra (2014b).

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1 Introduction

1.1 Background and aims

In Switzerland, the Nuclear Energy Law requires the disposal of all types of radioactive waste in deep geological repositories (KEG 2003). The Swiss Radioactive Waste Management Program (Nagra 2008a) foresees two types of deep geological repositories: a high-level waste repository (HLW repository[1]) for spent fuel (SF)[2], vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW), and a repository for low- and intermediate-level waste (L/ILW repository[3]). The procedure for selecting the site or sites[4] for the deep geological repositories is specified in the concept part of the Sectoral Plan for Deep Geological Repositories[5] (SGT, BFE 2008). The Sectoral Plan foresees a selection of sites in three stages, the third of which leads to a General Licence Application procedure that defines both the sites and the main features of the repositories.

In SGT Stage 1, Nagra proposed geological siting regions for the HLW repository and the L/ILW repository based on long-term safety and engineering feasibility criteria (Nagra 2008b). These proposals were later evaluated by the responsible federal authorities and their experts, who came to a positive conclusion (ENSI 2010a, KNE 2010, KNS 2010). In 2011, all proposed geological siting regions were formally approved by the Swiss Government (BFE 2011).

In SGT Stage 2, the overall objective is twofold: (i) to select at least two geological siting regions for each repository type for further geological investigations in SGT Stage 3; and (ii) to identify suitable locations for the surface facility in the geological siting regions identified in SGT Stage 1, which is carried out together with the regional participation bodies.

The selection of geological siting regions for further investigation in SGT Stage 3 is based on a formal safety-related comparison. This comparison follows the specifications in ENSI (2010b) and ENSI (2013); and is documented in the overarching technical report for SGT Stage 2 (Nagra 2014a). The safety-related comparison is based on so-called provisional safety analyses for deep geological repositories in the different geological siting regions.

According to ENSI (2010b), the main objectives of the provisional safety analyses are:

- to show that calculated individual dose rates for a deep geological repository in a given siting region are below the regulatory protection criterion 1 of 0.1 mSv per year, which is specified, along with the general requirements for the safety case of a deep geological repository, in ENSI (2009a),
- to demonstrate the post-closure safety performance and long-term behaviour of the individual elements of the barrier system of a deep geological repository,
- to provide input to the safety-related comparison of the geological siting regions by means of so-called characteristic dose intervals, and
- to show indication about the scope of further geological investigations in SGT Stage 3.

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1 In German: "HAA-Lager".

2 According to current legislation, spent fuel is classified as radioactive waste.

3 In German: "SMA-Lager".

4 It will be decided at a later stage whether the two repositories are to be implemented at different sites or at the same site (combined repository).

5 In German: "Sachplan geologische Tiefenlager (SGT)".

These objectives require the quantitative modelling of radionuclide release from the barrier systems in the geological siting regions. According to ENSI (2010b), this modelling should be based on the realistically to be expected evolution of the repository systems under consideration. It is thus confined to the reference scenario of radionuclide release from the geological repository systems, which is the release of dissolved radionuclides along the groundwater pathway under the premise that the engineered barriers function correctly. Because this modelling activity also involves the calculation of an individual radiological (effective) dose rate, it is in the following referred to as dose calculations for the provisional safety analyses or, in short, dose calculations. Within the reference scenario, a reference case is analysed, along with variant cases that explore the sensitivity to different processes and parameters.

This report describes in detail and comprehensively the models and computer codes applied in the dose calculations and the general modelling approach adopted. An overview of the scientific basis for the dose calculations is documented in Nagra (2014b), where the results of these calculations are also presented.

The present report provides additional information that would be needed to reproduce independently the results of the dose calculations in Nagra (2014b). However, it does not describe other models and modelling activities that are used to justify conceptual assumptions or to provide input parameters to the dose calculations. Such information is contained in Nagra (2014b) and references therein.

1.2 Description of the barrier systems

The post-closure safety of the repository systems to be compared in SGT Stage 2 relies upon a system of nested, passive engineered and geological barriers, which complement one another. Fig. 1-1 schematically illustrates the barrier systems for the different waste types. The individual elements of the barrier systems are the waste matrices, the disposal canisters / containers, the materials used for backfilling and sealing of the underground structures, and the host rock along with other geological formations that may provide an additional geological barrier (confining units). In the following paragraphs, an overview of the reference concept for the barrier systems is given so as to provide the basis for the content of this report.

Each element of a given barrier system performs one or several post-closure safety functions, which are: (i) physical separation of radioactive materials from the human environment, (ii) long-term stability of the barrier system, (iii) containment of radionuclides in disposal canisters / containers, (iv) delayed release of radionuclides from the waste matrices, (v) retention of radionuclides within the barrier system and (vi) other processes that contribute to low radionuclide concentrations in the biosphere (see Nagra 2014b).

The overall geological situation ensures the long-term stability of the barrier systems over the so-called time frame for safety assessment, which is the main period of concern from the perspective of post-closure safety and which was defined in Nagra (2008b) based on the decrease in radiological toxicity that occurs over time. The time frames for safety assessment extend to 100'000 years for the L/ILW repository and to one million years for the HLW repository.

On arrival at the surface facility of a deep geological repository, the radioactive materials to be emplaced in the repository will be in the following forms:

- Spent fuel (SF), consisting of single fuel assemblies (FAs), which integrate a large number of irradiated fuel rods (100 to 200). The fuel rods consist of stacks of cylindrical pellets contained in a zirconium alloy (Zircaloy) cladding, along with other structural materials consisting mainly of steel alloys. The pellets are composed of ceramic uranium oxide (UO_2) or a blend of UO_2 and PuO_2 (MOX).

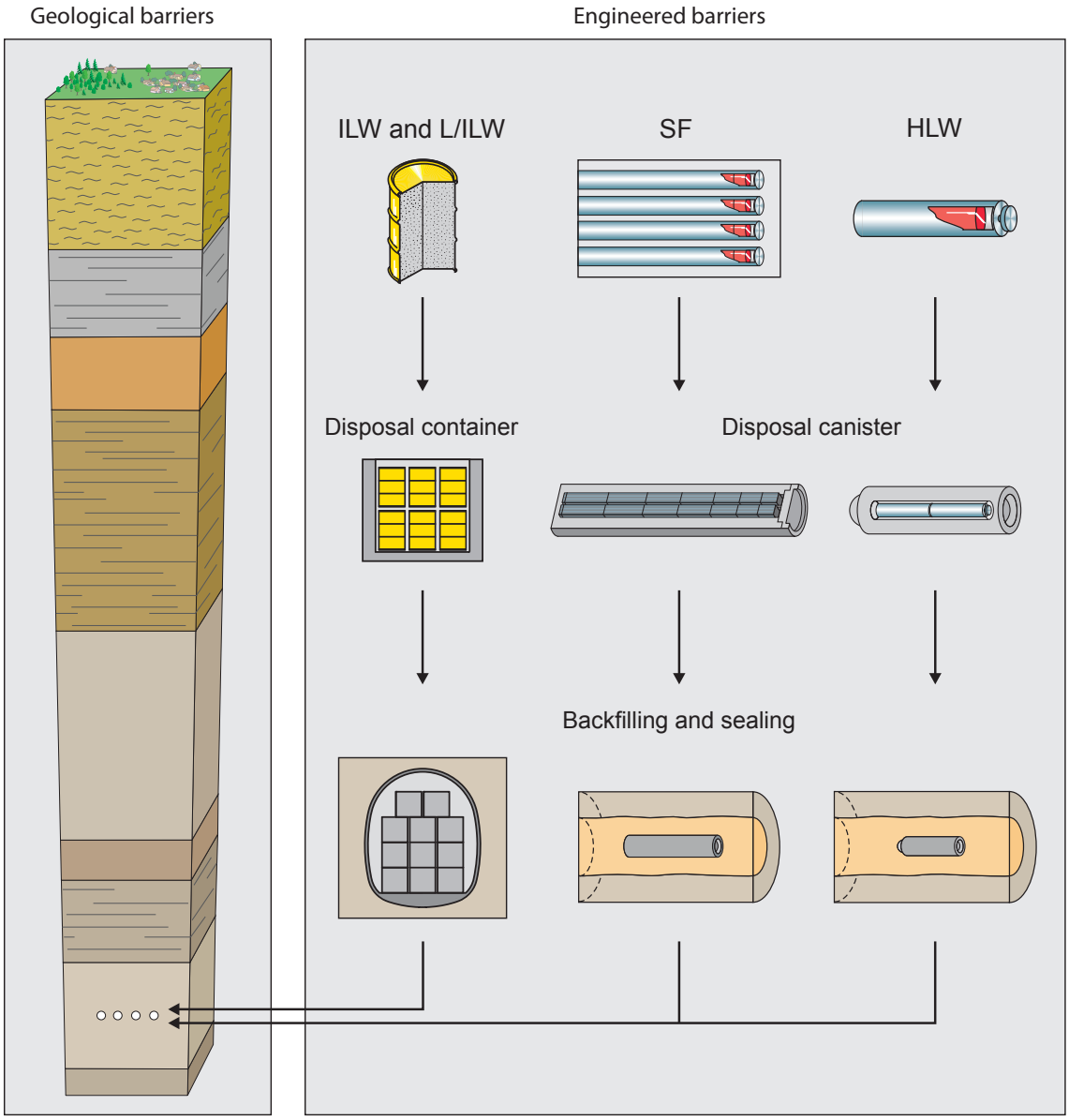

Fig. 1-1: Schematic illustration of the barrier systems for the different waste types.
Not drawn to scale. The emplacement rooms in the left picture do not correspond to any specific repository type or layout.

- Vitrified high-level waste (HLW), incorporating radionuclides in a homogeneous boro-silicate glass matrix within a thin stainless steel fabrication flask.
- Intermediate- and low-level waste (ILW / LLW or L/ILW), containing much lower activity than SF or HLW, with radionuclides embedded in a cement matrix or, in some cases, in a bitumen, polystyrene or borosilicate glass matrix. The waste matrix is usually packaged in steel drums and / or concrete containers.

A broad description of the properties of the radioactive waste to be disposed of and the differences between the individual waste types from the point of view of post-closure safety analysis is given in an appendix of Nagra (2014b).

In the surface facility, spent fuel assemblies and fabrication flasks with HLW are loaded into disposal canisters, which, according to the current reference concept, are fabricated of carbon steel. The disposal canisters are about 5 (SF) and 3 (HLW) meters long. They have a diameter of about 1 m (SF) or 0.7 m (HLW), and a wall thickness of about 14 cm (Patel et al. 2012).

In the case of the HLW repository, the underground facilities will be constructed in Opalinus Clay at a depth of a few hundred metres below the ground surface. They include a series of dead-end emplacement rooms for SF and HLW with initial diameters of about 2.5 m and lengths ranging from 300 m up to 1'000 m. The disposal canisters will be transported underground and emplaced within these tunnels. According to the reference concept, the canisters will be emplaced co-axially with respect to the tunnel walls on pedestals of compacted bentonite blocks. Immediately after emplacement, the respective tunnel section will be backfilled with highly compacted bentonite granules. The bentonite blocks and granules together form a protective mechanical and chemical buffer around the disposal canisters. The spacing between two individual canisters will be about 3 m. There is currently no requirement to have separate emplacement rooms for disposal canisters with different waste types, thus a mixed emplacement of SF and HLW is assumed in the following.

The current reference concept also includes a liner along the SF / HLW emplacement rooms. After every 10th canister or so, the liner is interrupted by an intermediate seal, which ensures direct physical contact between the bentonite backfill and the Opalinus Clay host rock, thus interrupting potential preferential water flow and solute transport pathways along the liner (see Nagra 2010a). Shortly after an emplacement room has been completely filled, a final seal consisting of highly compacted bentonite granules will be installed.

Long-lived intermediate-level waste (ILW) will be packaged in concrete disposal containers of standard size in the surface facility of the HLW repository. After transport to the underground facilities, the disposal containers will be stacked in dead-end emplacement caverns[6] of about 7 m width and which are supported by concrete lining (see Section 5.3). The remaining void spaces will be backfilled with a specifically designed mortar and eventually the caverns will be sealed. The current reference concept foresees a gas-permeable seal at the end of each ILW emplacement cavern.

The concept for waste emplacement in the L/ILW repository is in many ways identical to that of the ILW part in the HLW repository. One major difference concerns the size and shape of emplacement caverns, which will depend on the specific properties of the chosen host rock at a given site. Opalinus Clay is the only candidate host rock for the HLW repository, but, for the L/ILW repository, there are also other candidates. Although all potential host rocks for the L/ILW repository show – at least partially – high clay mineral content (consolidated clay rocks and marl) and / or low hydraulic conductivity, geotechnical conditions may vary between the candidate host rocks as well as between different sites, resulting in different constraints on the dimensions of the caverns. Furthermore, the extent of homogeneous rock blocks with favourable confinement properties (called the host rock in its strict sense) may vary between potential sites and between host rocks. As a result, the exact size and shape of the emplacement rooms can only be defined at a later stage. For the present dose calculations, two types of L/ILW cavern are assumed. For host rocks that provide relatively large homogeneous rock blocks suitable for waste emplacement, a medium sized cavern of type K09 is assumed. It has a width of about 10 m and a height of about 13 m. For other host rocks, a smaller cavern of type K04 with a width of about 7 m and a height of about 10 m is assumed. The reference length of an L/ILW emplacement cavern is set to 200 m (see Section 5.3).

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6 Emplacement rooms for ILW and L/ILW are sometimes also termed caverns in the present report.

The underground facilities of both the HLW repository and the L/ILW repository consist of:

- the main facility, i.e. the emplacement rooms, in which the radioactive waste will be emplaced,
- the pilot facility with representative amounts of the radioactive waste,
- a test area, also called the underground research laboratory (URL),
- a central area, and
- various types of seals at different locations within the underground structures.

The emplacement rooms will be arranged in disposal areas[7], the final size and shape of which will be determined later based on in-situ geological conditions. In this report, the term emplacement area is used as a synonym for disposal area.

Access to both repositories will be provided, during construction and operation, by a ramp, by shafts or by any combination of these. As mentioned in Section 1.1, the dose calculations are based on the reference scenario for radionuclide release, in which the engineered barriers function correctly, thus virtually no radionuclide release occurs along the underground access structures. Figs. 1-2 and 1-3 show example layouts of the HLW repository and the L/ILW repository, respectively.

1.3 Organisation of this report

The present report is the successor of the Models, Codes and Data Report from the Opalinus Clay project (Nagra 2002a), although its scope is rather different, which is reflected in differences in the structure and contents of the two reports. In particular, the Models, Codes and Data Report (Nagra 2002a) contains in its main chapters detailed descriptions of each of the calculation cases for the safety case of project Opalinus Clay. In the framework of the dose calculations for SGT Stage 2, information about the individual calculation cases, including the definition of site-specific concepts for radionuclide transport in the geosphere and the most relevant input parameter values, is contained principally in Nagra (2014b).[8] Furthermore, in Nagra (2002a) the generic conceptual models and codes were described in an appendix, whereas, in the current report, the generic conceptual models and codes are provided in the main text.

Another main constituent of this report is a detailed description of the general modelling approach to the dose calculations. The general modelling approach comprises all generic assumptions made and procedures adopted to model radionuclide release and transport in the engineered and geological barriers within the given scenario. This includes, for example, the topics of code selection, code application and code interfacing.

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[7] In German: "Lagerkammerbereich".

[8] The complete set of code-specific input parameter values for the individual calculation cases and the detailed results are also documented in the electronic input data and results application (EDR, Nagra 2014d).

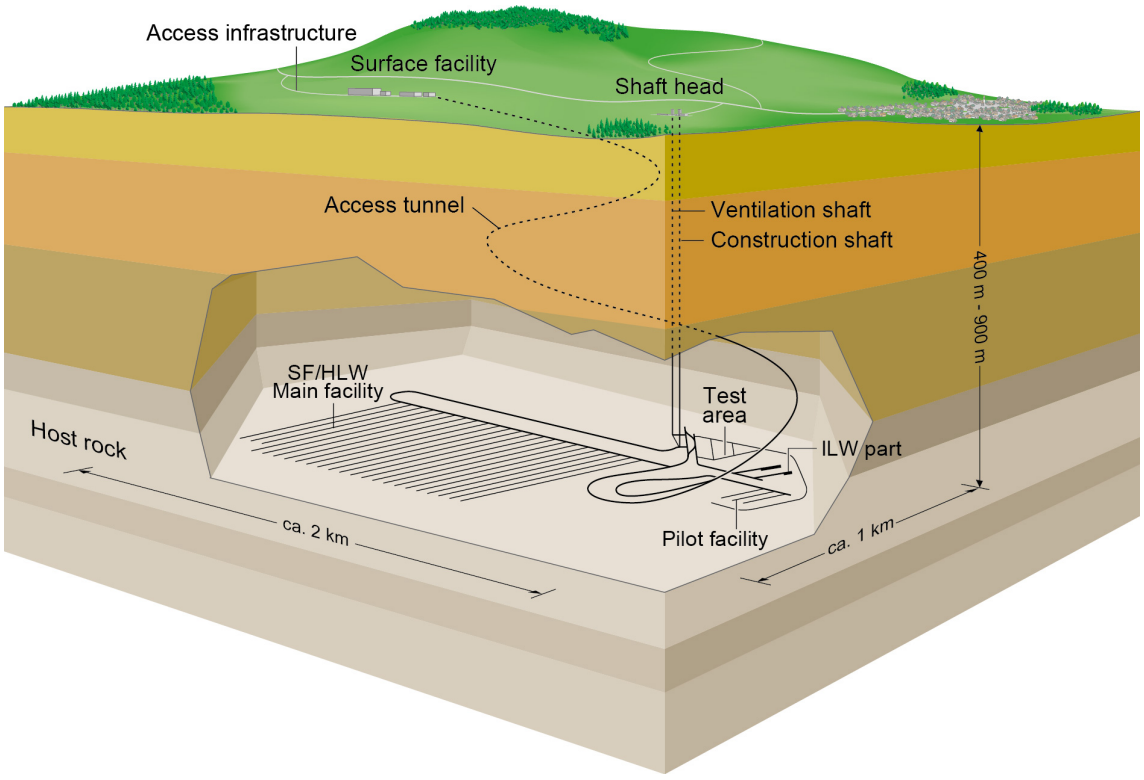

Fig. 1-2: Example layout of the HLW repository with its main features.
Not drawn to scale.

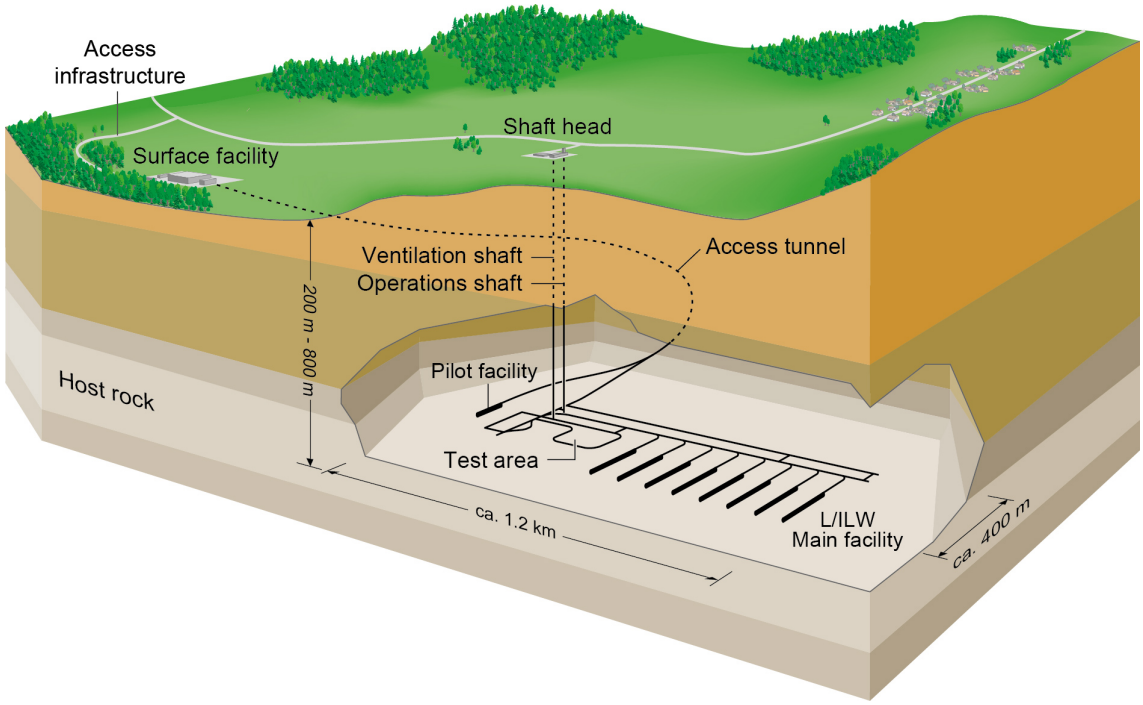

Fig. 1-3: Example layout of the L/ILW repository with its main features.
Not drawn to scale.

Although the general modelling approach is largely based on the general modelling approach used in SGT Stage 1 (see e.g. Nagra 2008b), there are a number of differences resulting from a more detailed understanding of the geological conditions in the individual geological siting regions, from new capabilities that have been added to the safety assessment codes and from certain requirements arising from the overall objective of SGT Stage 2; i.e. the comparison of repository systems in different geological siting regions.

It is further important to note at this point that, in the context of the provisional safety analyses for SGT Stage 2, the barrier system of a deep geological repository comprises only the engineered and geological barriers. The biosphere is not considered as part of that barrier system. For this reason, biosphere modelling is described in a separate chapter in the present report.

The report is structured as follows:

- Chapter 2 familiarises the reader with the overall modelling process in the context of the dose calculations, followed by an overview of the general modelling approach adopted. Finally, it introduces the computer codes that are used for the dose calculations and sets out general code verification principles.
- Chapter 3 presents generic concepts of radionuclide release and transport in the engineered and geological barriers within the given scenario and summarises their relationship to the processes and parameters that are relevant in the context of the current siting process and which are summarised in Appendix A. It shows how these concepts are transformed into mathematical equations and describes the safety assessment codes that solve these equations numerically.
- Chapter 4 provides an overview of the concepts of radionuclide transfer and radiation exposure in the biosphere as well as their mathematical formulation and their implementation in specific codes.
- Chapter 5 describes in detail the application of the safety assessment codes for the engineered and geological barriers to the dose calculations for the provisional safety analyses (general modelling approach). The topics of code selection, code application and code interfacing form an integral part of this discussion.
- Appendix A lists the processes and parameters that are of relevance in light of the on-going site-selection process. This list is a translation of the original list in Nagra (2014b).
- Appendix B describes how the numerous numerical calculations performed to analyse the calculation cases are managed. This includes an overview of the calculation management process and of the software tools used to facilitate this process.
- Appendix C gives a summary of the quality assurance measures related to the development of the safety assessment codes and to the execution of the modelling work.
- Appendix D lists the symbols and abbreviations used in this report. It also shows the links between individual input parameters of the codes and the relevant processes and parameters listed in Appendix A.

2 Overview

This chapter gives an overview of the modelling process in the context of the dose calculations (Section 2.1) and of the general modelling approach to the dose calculations (Section 2.2). It further presents the safety assessment codes applied and discusses some general aspects with regard to code verification (Section 2.3).

2.1 Modelling process

The modelling process of the dose calculations for the provisional safety analyses in SGT Stage 2 is illustrated in Fig. 2-1 and explained in more detail in the following paragraphs.

The basic information for the dose calculations consists of

- the general and specific regulatory requirements given in ENSI (2009a), ENSI (2010b) and ENSI (2013);
- the comprehensive list of relevant processes and parameters for a deep geological repository from the perspective of the current site selection process (see Appendix A);
- the findings of detailed system analyses that provide insight into the initial state and performance of the barrier systems at closure and how the performance will evolve over time as the physical and chemical environments change;[9]
- general concepts and input data, such as the radionuclide inventory, the corresponding repository configurations and site-independent geological information; and
- geological information specific to the individual siting regions.

All these types of information are presented and discussed in Nagra (2014b), with references to other more detailed reports.

Starting from the basic information outlined above, generic concepts of radionuclide release from the solid waste forms, radionuclide migration and radiation exposure are developed (see right part of Fig. 2-1 and Sections 3.1 and 4.1). These concepts are generic in the sense that they are not specific to a given barrier system, to a given geological siting region or to a given biosphere system in a potentially affected region. In addition, they incorporate only those processes that are most relevant to radionuclide release and migration in the barrier / biosphere system as well as to radiation exposure in the biosphere. The relative simplicity of the generic concepts thus contrasts with the extensive scientific understanding that underpins the formulation of these concepts.

The generic concepts are expressed as (generic) mathematical models. These generally take the form of sets of partial differential equations, complemented with the requisite initial conditions, boundary conditions and possibly complementary constitutive relationships. Sections 3.2 and 4.2 describe the most important mathematical models and highlight the link between the model parameters in the individual equations and the relevant processes and parameters listed in Appendix A.

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[9] This insight also provides the basis for the argumentation as to why individual processes and parameters do or do not have to be addressed explicitly in the dose calculations for a given barrier system. Furthermore, it provides guidance to repository design and to the allocation of wastes to the various repository types (see Nagra 2014b).

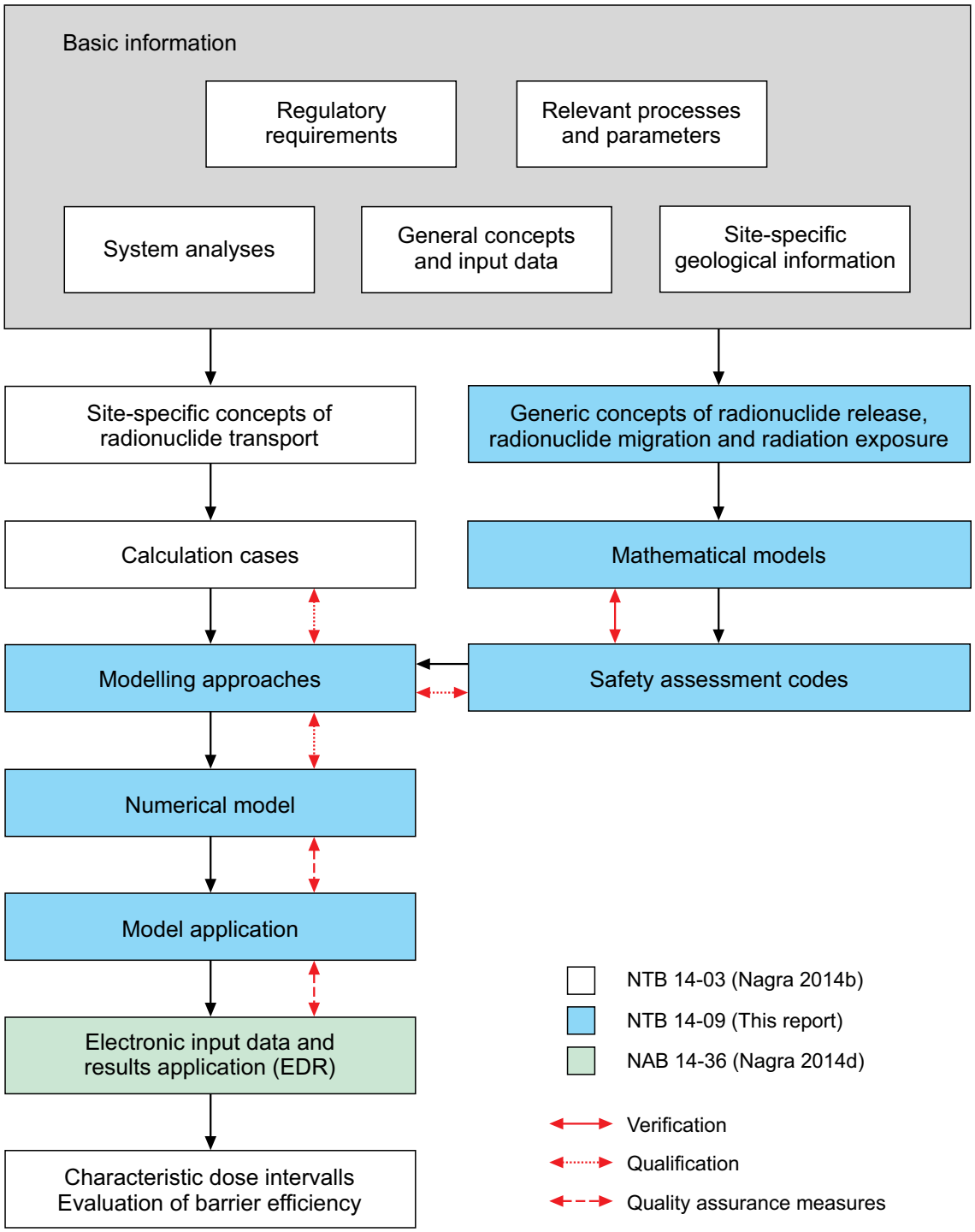

Fig. 2-1: Illustration of the modelling process of the dose calculations for the provisional safety analyses in SGT Stage 2.

Black arrows indicate workflow, red arrows are checks of different types. See also Fig. 4.1-1 in Nagra (2014b).

In order to solve the mathematical models, numerical techniques are employed and implemented in generic safety assessment codes. The use of generic codes, rather than codes tailored to a specific geological siting region or barrier system, provides the flexibility needed for the relatively large number of dose calculations to be carried out in SGT Stage 2. In addition, it minimises any additional bias that would be introduced if site-specific modelling techniques were applied (see Section 5.1). The description of the safety assessment codes and the generic concepts and mathematical models on which they are based forms the subject of Chapters 3 and 4 of the present report.

The safety assessment codes must provide solutions that have sufficient numerical accuracy. The assessment of the correctness of computer software and of the numerical accuracy of the solution to a given mathematical problem is termed verification. Verification is discussed further, in general terms, in Section 2.3 of the present chapter and the most important verification steps for the individual safety assessment codes are summarised in Chapters 3 and 4.

The safety assessment codes are applied to a range of calculation cases. The calculation cases themselves are based on site-specific concepts of radionuclide transport for the barrier systems under consideration. These concepts reflect different possible geological situations and evolutions, which may vary, e.g. in the extent of the effective containment zone (as defined in the discussion of model boundaries in Section 2.2.2) and in the properties of transport pathways. Both the site-specific concepts of radionuclide transport and the derivation and classification of individual calculation cases are important elements of Nagra (2014b).

The modelling approaches adopted for each calculation case have both generic aspects and aspects that are specific to the geological siting region, the barrier system and / or the calculation case at hand. Together, these modelling approaches provide a comprehensive description of how the barrier system is to be modelled for the calculation case at hand using the available codes. They describe, for example, the degree to which the geometry of the emplacement room and its immediate environment is simplified (e.g. 3D vs. 1D representation) and decisions as to how specific processes and parameters are handled, if this is not part of the calculation case definition itself.

The set of generic modelling approaches, taken together, is termed the general modelling approach. It is described in detail in Chapter 5 and summarised in the following Section 2.2. Complementary site-specific and / or case-specific modelling approaches are discussed principally in Nagra (2014b).

The definition of the modelling approaches is linked to the selection of appropriate safety assessment codes and suitable input data, which together form one or several numerical models for each calculation case. It is therefore evident that the modelling approaches are constrained, to some extent, by the available codes. On the other hand, if the available codes do not adequately handle the required processes and parameters, then this can be a driver for further code development. This interplay between the requirements on modelling and the safety assessment codes is one aspect of qualification.

Qualification in general terms is the process of showing that the model – or the set of models – adopted represents adequately all phenomena relevant to the calculation case at hand, and is thus fit for purpose[10]. Thus, the model must be qualified, particularly with respect to phenomena and concepts included in the chosen modelling approaches.[11] The modelling approaches must themselves be qualified with respect to the calculation-case definition, the selected safety assessment codes and the basic information that underpins these two.

The individual numerical models may represent different parts of the barrier system. After a numerical model has been set up, it is run and post-processed on a high-performance Linux cluster in an automatic and efficient manner. Note that running the computer codes chosen to analyse a specific calculation case using an appropriate set of input parameters is here termed a model run, but is also commonly referred to as model execution, model application or simply calculation. All input files and results are stored in an electronic input data and results application (EDR), from which the results can be extracted as figures and / or tables for further use. Details of the actors, roles, activities, procedures and tools involved when running the models are compiled in Appendix B. The respective quality assurance measures are summarised in Appendix C.

For each calculation case, the evolution of an individual effective dose rate resulting from radionuclide release from the barrier system to the biosphere is calculated. The results of the dose calculations provide input to the safety-related comparison of siting regions by means of the earlier mentioned characteristic dose intervals and also serve to evaluate the post-closure safety performance of the barrier systems in a quantitative manner. These steps are documented in Nagra (2014b).

2.2 General modelling approach

The general modelling approach adopted in the dose calculations as part of the provisional safety analyses for SGT Stage 2 is broadly the same as that adopted in SGT Stage 1 (see Nagra 2008d and 2010a). Nonetheless, some differences exist, mainly as a result of improved knowledge about the geological conditions in the geological siting regions, the development of new computer codes or the refinement of existing codes, and slight differences in the modelling requirements for SGT Stage 2 compared with Stage 1. The general modelling approach is described in detail in Chapter 5. The following paragraphs serve as a summary of this detailed description.

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[10] The definition of qualification, in contrast to model validation, reflects the fact that a key issue in repository safety assessment is the identification of phenomena that may affect the disposal system over prolonged periods of time (typically in the order of a million years), some of which may not be apparent in experiments or observations conducted over much shorter periods. Models can therefore not be validated in a strict sense. This has long been acknowledged internationally and has recently been confirmed in a recent OECD/NEA publication (NEA 2012). Note that other organisations use terms such as "code validation" and "confidence building", which basically mean the same as the term qualification, as used in the present report (see e.g. POSIVA 2012).

[11] In this context, ENSI (2009a) states that a "justification that the models used in the calculations are applicable to the situation considered" is required.

2.2.1 Requirements

The general requirements on safety assessment of a deep geological repository are set out in ENSI (2009a). Additional requirements that are specific to the provisional safety analyses in SGT Stage 2 are given in ENSI (2010b) and ENSI (2013). Complementary to these regulatory guidelines, some further requirements on modelling aspects of the dose calculations are derived from the overall objective in SGT Stage 2, namely the safety-related comparison of different geological siting regions (see Section 5.1):

1. Results to be compared (i.e. results for the same repository type or the same part of a repository type) must be based on the same general modelling approach and be calculated with the same set of codes.
2. Modelling approaches and parameter values that are likely to underestimate radiological consequences should be avoided.
3. Case-specific modelling approaches should be consistent with the general modelling approach.
4. Highly conservative modelling approaches and parameter values should be avoided, as these may mask prevailing differences between the geological siting regions.

In carrying out the dose calculations for the provisional safety analyses in SGT Stage 2, an optimum balance is sought between these complementary requirements.

2.2.2 Definition of the model system

The model system is tailored to the release scenario to be investigated, which is the release of dissolved radionuclides along the groundwater pathway under the premise that the engineered barriers function correctly. This means, in particular, that no radionuclide transport along the underground structures of a geological repository needs to be considered in the context of the dose calculations. The model system thus only includes the emplacement areas of the repository systems under consideration, along with the adjacent geological environments. Since the biosphere is not considered a part of the barrier system, it is treated as a separate, independent model system (see Section 2.2.5).

The model domain of the barrier system is further subdivided into the near field and the geosphere. The near field includes an individual SF or HLW disposal canister, together with its surrounding bentonite buffer; or an individual ILW or L/ILW emplacement room.[12] It also includes in both cases a limited region of the surrounding host rock. The geosphere comprises the part of the host rock that is not affected, or only slightly affected, by the repository and – depending on the geological situation considered – additional overlying and underlying rocks that contribute to the confinement of radionuclides. This domain is called the effective containment zone (ECZ, see the discussion of model boundaries, below). The modelling of radionuclide release and transport within the ECZ is further described in the following paragraphs, with more specific aspects concerning the near field and the geosphere presented in Sections 2.2.3 and 2.2.4, respectively.

[12] The calculated results are then multiplied by the number of disposal canister or emplacement rooms, respectively.

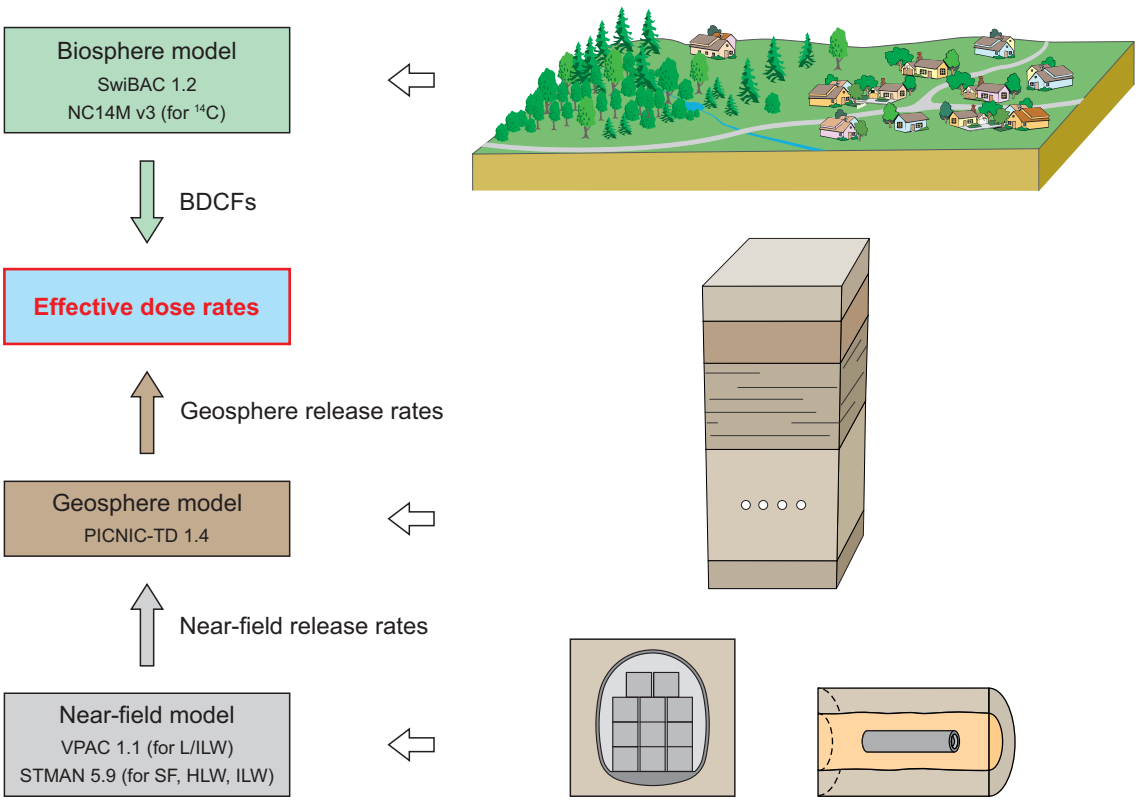

Fig. 2-2: The model chain and the individual codes used in the dose calculations.
BDCFs: Biosphere dose conversion factors.

The near field and the geosphere are modelled consecutively and with dedicated computer codes, while respecting the requirements outlined in the previous section. The calculated release of radionuclides from the near field provides the source term for radionuclide transport modelling in the geosphere. Geosphere release rates are not, however, used directly as a source term for biosphere modelling. Rather, the biosphere model is used to evaluate biosphere dose conversion factors (BDCFs), which convert geosphere release rates to effective dose rates, as explained further in Section 2.2.5. The entire set of codes, together with the information flows between them, is often referred to as the model chain, which is illustrated in Fig. 2-2.

As mentioned further above, the horizontal extent of the model system is confined to the individual emplacement areas of a deep geological repository. According to the current repository concepts, the HLW repository consists of the SF / HLW emplacement area plus the ILW emplacement area. The L/ILW repository comprises only the L/ILW emplacement area. A combined repository would include all of these types of emplacement area. Each emplacement area is composed of a number of emplacement rooms, which are assumed to be horizontally orientated. The near-field release from each emplacement area is calculated as the sum of the individual near-field releases from the different waste types within that area. Similarly, the total radionuclide release from the near field (or geosphere) is calculated by summing the near-field (or geosphere) releases from all emplacement areas belonging to the considered repository system.

The vertical extent of the model system for each emplacement area is set in such a way that it contains the full extent of the geological environment that is considered to effectively contribute to the confinement of radionuclides (effective containment zone, ECZ). This extent may be specific to a given geological situation, depending on the barrier efficiency of individual transport paths within the host rock and / or the confining units.

The individual rock units[13] within the ECZ are mostly conceptualised, for modelling purposes, as horizontal, homogeneous porous media[14], which may, where appropriate, be assigned anisotropic water flow and solute transport properties. Because of the low hydraulic conductivity of the rock units within the ECZ – in comparison with the hydraulic conductivity of the adjacent rocks – the ambient hydraulic gradient across the ECZ and the natural water flow through the ECZ are, to a first approximation, both orientated perpendicular to its layered structure (if this exists), i.e. perpendicular to the emplacement areas and their constituent emplacement rooms.

The side boundaries of the model system are, in the reference case and in most other cases, assumed to be impermeable to water and radionuclides[15]. Zero radionuclide concentration boundary conditions are imposed at the upper and lower model boundaries, which is conservative. The radionuclides can move across these boundaries, which are referred to as release points, even though they may have significant lateral extent. An instantaneous transfer of radionuclides is assumed to occur from these release points to the same biosphere system.

It is fundamental to note that the individual radioactive waste packages and waste types are – in the context of the current site selection process – not assigned to a particular location within an emplacement area or an emplacement room. Rather, average inventories are assigned to all canisters or packages containing a given waste type (or group of types with similar characteristics). The pilot facility is not explicitly modelled. Instead, its inventory is added to those of the emplacement areas representing the main facility of the repository. The list of radionuclides and stable isotopes considered in the modelling is restricted to the so-called safety-relevant nuclides, which have been identified in a precursory analysis and which contains the same radionuclides and stable isotopes that were considered in SGT Stage 1 (see Nagra 2008b).

The modelling period is extended to 10 million years after closure, i.e. well above the safety-relevant time frames for the HLW and L/ILW repositories (see Section 1.2), with the aim of better understanding the safety performance and effectiveness of the different barriers at the end of the respective safety-relevant time frames. In performing the analyses, it is hypothetically assumed that the conditions in the barrier systems at the end of the respective safety-relevant time frames prevail up to the end of the modelling period, even though the evolution of the repository barriers is subject to considerable and increasing uncertainties at such times.

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[13] In Nagra (2014b), the term "lithofacial unit" is used for a given part of the geosphere that is assumed to have homogeneous properties with respect to water flow and radionuclide transport. In this report, the term "rock unit" is used as a synonym.

[14] In case of a geological medium interspersed with joints, a homogeneous porous medium with equivalent flow and solute transport parameters is considered in the near-field models. The joints may, however, be explicitly represented in the geosphere models.

[15] The reference scenario assumes that the emplacement rooms are properly sealed so that horizontal water flow and transport of dissolved radionuclides along the repository tunnel system are negligible. Transport along the SF / HLW emplacement rooms is prevented through the construction of intermediate seals. The hypothetical effects of ineffective seals on radionuclide transport in solution are analysed in Nagra (2014c). An alternative modelling approach for radionuclide transport across the side boundaries of the modelled domain along localised water-bearing tectonic-structural elements is described in Section 5.4.3.

The processes in the barrier systems considered explicitly in the framework of the dose calculations for SGT Stage 2 are:

- radioactive decay and ingrowth,
- instantaneous and / or gradual release of radionuclides and stable isotopes from the waste matrices to solution,
- saturated groundwater flow, along with advective[16] and diffusive transport of radionuclides and stable isotopes in solution, and
- temporary immobilisation of radionuclides and stable isotopes by sorption on solid-phases and / or by precipitation.

These processes are well supported by the current scientific knowledge, as described in Nagra (2014b) and references therein. The potential effects of unsaturated conditions in the near field on the transport of dissolved radionuclides through the barrier system are not explicitly addressed by the dose calculations. They are, however, discussed in the context of system analyses in the main report. Release of radionuclides in gaseous form is not included in the dose calculations, since this transport mode is outside the scope of the reference scenario.

A more detailed overview of the model system for the engineered and geological barriers is given in Section 5.2.

2.2.3 Near field

The most important conceptual assumptions for calculating radionuclide release from the solid waste forms and solute transport in the near field are summarised briefly below. Full details are given in Section 5.3.

Low- and intermediate-level waste (L/ILW)

- In order to account for the time needed to saturate the near field and for the radionuclides to become mobile, the calculations begin after an assumed containment period of 100 years. During this period, the radionuclide inventory is altered by radioactive decay and ingrowth.
- At the end of the assumed containment period, radionuclides are assumed to be spatially uniformly distributed within the emplacement rooms. They are also distributed between sorbed phases and solution, with dissolved radionuclides assumed to be fully mobile. This means that immobilisation due to incorporation of radionuclides in the waste matrices or possible confinement within tight waste packages is conservatively omitted. An exception, however, is the assumed limited release rate of C-14 incorporated in radio-activated metallic components; the release of incorporated C-14, presumed to be present as organic species, is assumed to take place at a constant rate as these components corrode.
- Radionuclide transport in the near field is assumed to occur by advection and diffusion, taking into account sorption, dispersion, radioactive decay and ingrowth, as well as the site-specific conditions in the host rock (e.g. the presence of tectonic-structural elements with increased permeability etc.).

[16] The advective component also includes the phenomenon of mechanical dispersion due to the effects of heterogeneity on advective transport.

Spent fuel and vitrified high-level waste (SF and HLW)

- All SF and HLW disposal canisters are assumed to breach simultaneously[17], allowing the release of radionuclides to begin. The canisters are conservatively assigned a 10'000 years' lifetime - a value that is expected to be greatly exceeded in reality (Patel et al. 2012). The conservative lifetime is used because of current uncertainties in the rate and mechanisms of corrosion, e.g. the possibility of pitting corrosion. Prior to canister breaching, the radionuclide inventory is altered by decay and ingrowth.
- The release of radionuclides and relevant stable isotopes from the waste matrices to solution is assumed to begin at the assumed time of canister breaching, the release rate being constrained by the dissolution rate of the SF and HLW matrices, the corrosion rate of the SF cladding and the limited solubilities of certain elements. An instant release fraction is taken into account for some radionuclides and stable isotopes.
- Radionuclides are assumed to diffuse from the interior of the breached canister into the bentonite buffer, from where they diffuse radially towards the buffer outer boundary, taking into account sorption, radioactive decay and ingrowth and the solubility limits of certain elements.
- Chemical interactions between the tunnel liner and the bentonite buffer, as well as between the corroded disposal canister and the bentonite buffer, lead to mineral alterations in the bentonite in the vicinity of both contact surfaces. These are addressed in the assignment of specific transport parameter values within these regions.

Long-lived intermediate-level waste (ILW)

ILW is modelled in the same way as L/ILW, with the exception that, at the end of the assumed containment period, radionuclides may be precipitated if their concentrations exceed the respective solubility limits, in addition to being sorbed or present in aqueous solution.

Any disturbed zone that may exist in the host rock around the emplacement rooms due to the presence of the repository (e.g. fractures and chemical alteration) is not explicitly modelled. It is, however, taken into account in the derivation of the transport path lengths or of transport parameter values for the geosphere. In all near-field models, the total (positive) radionuclide flux into the host rock at a distance of 1 m on all sides of the emplacement rooms is defined to be the radionuclide release rate from the near field (See discussion in Section 5.3.5). This radionuclide flux is then used as source term for the subsequent geosphere model.

The VPAC 1.1 code, described further in Section 3.3, is used to model nuclide release and transport in the L/ILW repository near field. This code calculates two- or three-dimensional groundwater flow and radionuclide release, retention and transport in homogeneous or heterogeneous (fractured) water-saturated porous media, and is therefore appropriate for modelling the near field of the L/ILW repository, given the potentially more heterogeneous structure of the host rock. The various near-field release and transport calculations for the HLW repository near field are performed using the code STMAN 5.9, which is described further in Section 3.4. This code calculates one-dimensional, radial diffusive transport in the engineered barrier system, as well as one-dimensional advection, dispersion and diffusion in an adjoining, low permeable host rock layer.

[17] This is a conservative assumption. In reality, a distribution of breaching times is expected, leading to some spreading of releases, which has the most significant effect on radionuclides with an inventory component that is rapidly released upon canister breaching.

2.2.4 Geosphere

The following paragraphs summarise briefly the most relevant generic conceptual assumptions for modelling transport of dissolved radionuclides in the geosphere. A complete description is given in Section 5.4.

The geosphere is modelled as a vertical sequence of horizontally-orientated, water-saturated rock units, each with homogeneous properties. Based on this representation and because of (i) the use of average inventories, (ii) the assumed homogeneous distribution of these inventories within each emplacement area / room, and (iii) the assumed impermeability of the side boundaries of the model system, radionuclide transport in the geosphere is taken to be one-dimensional and vertical. It occurs, however, in both directions (upwards and downwards), due mainly to the occurrence of diffusion.

Rock units are, in most cases, represented as homogeneous porous media (HPM). In a HPM, water flow is assumed to occur within a system of connected rock pores according to Darcy's law. At relatively high water flow rates, the transport of dissolved radionuclides takes place predominantly by advection and by the related process of hydrodynamic dispersion. At lower water flow rates, transport of radionuclides occurs mainly by diffusion. The retention of dissolved radionuclides due to sorption on solid phases is quantified using equilibrium distribution coefficients (K_d values). The values of these coefficients are based on scientific knowledge of mineralogy and pore water chemistry for each rock unit.

In a few instances, rock units may comprise discrete, small-scale water-bearing structures, and are thus modelled as fractured porous media. Different conceptualisations of the structures are possible, depending on their geometrical arrangements and other characteristics. In the framework of the present dose calculations, such rock units are modelled as regular, vertical, planar open fractures (i.e. without any fracture filling) embedded in a porous rock matrix, with diffusive exchange of radionuclides between the fractures and the rock matrix pore spaces (matrix diffusion)[18].

In the case of a large and steeply-dipping fault with distinct hydraulic properties, the rock adjacent to the fault is again represented as a homogeneous porous medium, or alternatively as a fractured porous medium, as described above. The faults themselves are modelled as large-scale fractures, using the same modelling approach as for small-scale fractures. It is further pessimistically assumed that the ambient hydraulic gradient across the ECZ is not reduced in the vicinity of faults.

All geosphere model calculations are carried out with the code PICNIC-TD 1.4, which is described in more detail in Section 3.5. The code calculates the transport of dissolved radionuclides along one-dimensional transport paths, termed "legs". The legs can be joined together to form a transport network. Legs usually correspond to individual rock units. They can represent either homogeneous, porous transport paths or fractured transport paths corresponding to discrete water-bearing structures such as fissures, joints or faults, with the possibility of diffusive exchange of radionuclides across the surfaces of these structures with the stagnant pore water of the adjacent rock matrix.

[18] In calculation cases that investigate the potential effects of colloid-facilitated transport in the fractures, matrix diffusion of sorbing radionuclides is inhibited in the model.

2.2.5 Biosphere

In the context of the provisional safety analyses for SGT Stage 2, the biosphere is taken to include a limited area of the terrestrial surface in which people that are most exposed to radionuclide releases from the barrier system are assumed to reside. Such areas are typically located in regions where discharge of deep groundwater from the geological siting regions occurs, since radionuclide concentrations in the environment are expected to be highest in these regions. The biosphere model system for each such area includes the vegetation, livestock and other fauna present, the atmosphere and surface waters and, below ground, the soils and an underlying near-surface aquifer. The potential radiation exposure of a representative person of the above-mentioned group is derived from the calculated radionuclide concentrations in the biosphere model, taking the most relevant exposure pathways into account.

For the more highly exposed individuals, an average present-day diet and present-day agricultural practices are assumed. A number of additional assumptions are also made to ensure that dose rates received by the representative person are not underestimated. However, care is taken that these assumptions are plausible and do not represent the potentially extreme habits of a single individual. Steady-state climatic and geomorphological conditions (temperature, precipitation rates, river systems etc.) that are typical of the surface conditions to be expected throughout the respective time frames for safety assessments of the different repository types are assumed in any individual biosphere calculation. In reference calculations for SGT Stage 2, present-day temperate climatic conditions are assumed. Other climatic conditions are investigated with alternative conceptual models[19] and / or alternative parameter values.

A terrestrial fresh-water ecosystem used for agricultural production is selected in reference calculations. Radionuclides released from the geosphere enter the biosphere as dissolved species in deep groundwater. A local aquifer in direct contact with a river is selected to be the recipient unit for deep groundwater that conveys radionuclides. To obtain the distribution of radionuclides within the biosphere region under consideration, a modelling approach is adopted whereby the biosphere is conceptually divided into a number of discrete compartments, namely:

- the rooting zone (top) soil of agricultural land,
- the near-surface (local) aquifer,
- the surface water,
- bed sediments associated with the surface water, and
- intermediate (deep) soil horizons between the aquifer and the rooting zone,

together with a small number of ancillary compartments.

The modelling approach to calculating radionuclide concentrations in the biosphere further consists of:

- transient (dynamic) modelling of processes with characteristic timescales of at least several years, which are mainly the physical transport processes between individual compartments representing e.g. the soil, aquifer and surface water body, and
- an equilibrium treatment of relatively rapid processes occurring on a timescale of around a year or less.

[19] For periglacial conditions, a more stylised modelling approach is adopted (see Chapter 4).

In each compartment, radionuclides are either dissolved in the aqueous phase or associated with solid materials. It is assumed that radionuclide concentrations in any given compartment are homogeneous. Radionuclides migrate between compartments in solution with fluxes of water and by vertical diffusion, as well as with fluxes of solid materials with which they may be associated. Some radionuclides can also migrate in the gas phase (see the description of the treatment of C-14 in Section 4.1.7).

Rapid processes, such as the exchange of radionuclides between water and solid materials, are represented within each compartment by an assumption of equilibrium. Similarly, an equilibrium approach is used to represent biological processes occurring in crops, livestock and humans, where accumulation and internal transport mechanisms are largely determined by cycles operating on annual or even shorter time scales.

The following radiation exposure pathways are considered:

- Consumption pathways:
  - drinking water,
  - freshwater fish,
  - meat, eggs, milk and dairy products, and
  - grain, green vegetables, root vegetables and fruit.
- Environmental exposures:
  - external irradiation, and
  - inhalation of radioactive dust and / or radioactive gas escaping from the top soil.

A key feature of radionuclide releases from deep geological repositories into the biosphere is that – for most radionuclides – they vary over timescales that are much longer than the timescales that characterise the most relevant transfer and accumulation processes in the biosphere. This observation leads to the possibility of assuming equilibrium with respect to the radionuclide concentrations in the different biosphere compartments and thus of calculating steady-state biosphere dose conversion factors (BDCFs) as a convenient way to convert radionuclide release rates from the geosphere into effective dose rates.

The biosphere model for SGT Stage 2 is implemented using the code SwiBAC 1.2, which is described in more detail in Section 4.3. SwiBAC evaluates the distribution of radionuclides in a terrestrial fresh-water ecosystem used for the production of food and water using the dynamic compartment modelling approach as summarised above. Based on the derived distribution of radionuclides, the potential exposure of humans is determined. SwiBAC provides, as output, time-varying radionuclide-specific annual individual effective dose rates, as well as the above-mentioned BDCFs.

The migration and distribution of C-14 in the biosphere is modelled using a code called the Nagra C-14 model (NC14M, v3). It provides, as output, effective parameters to be used in SwiBAC calculations to obtain effective dose rates or BDCFs for C-14.

2.3 Safety assessment codes and general verification aspects

For SGT Stage 2, the safety assessment codes described in Nagra (2002a) have been supplemented with the newly developed versatile performance assessment code, VPAC, and the biosphere model has been integrated in a more flexible code environment called SwiBAC. The functionality of the earlier versions of the codes STMAN and PICNIC has also been refined / extended, particularly with respect to the level of geometric detail that may be accounted for in

the near-field models, to the interfacing between near-field and geosphere models and to the way in which individual transport paths in the geosphere are linked together. The conceptual model concerning the dynamics of carbon in the biosphere system under consideration has also been extended and implemented in the code NC14M, which can be interfaced with SwiBAC.

Tab. 2-1 gives an overview of the safety assessment codes used in the dose calculations for SGT Stage 2. It shows the model domains for each code and, where applicable, the usage of earlier versions of each code in previous Nagra safety assessments. The codes and the underlying generic concepts and mathematical formulations are described in more detail in Chapters 3 and 4. The position of each code within the assessment model chain is illustrated in Fig. 2-2.

Tab. 2-1: Overview of safety assessment codes used in the dose calculations for the provisional safety analyses.

Model domain	**Waste category**	**Safety assessment code**	**Reference document**	**Use in earlier safety assessments**
Near field	L/ILW	VPAC 1.1	Holocher et al. (2008)	Successor of VPAC 1.0 used in SGT Stage 1
	ILW	STMAN 5.9	Robinson (2013)	Successor of STMAN 5.7 used in SGT Stage 1 and STMAN used in project Opalinus Clay
	HLW			
	SF			
Geosphere	-	PICNIC-TD 1.4	Robinson & Watson (2013)	Successor of PICNIC 2.4 used in SGT Stage 1 and PICNIC used in project Opalinus Clay
Biosphere	-	SwiBAC 1.2	Walke & Keesmann (2013)	Successor of TAME 3c, used in project Opalinus Clay and SGT Stage 1
		NC14M v3	Nagra (2013)	Newly developed code

Verification of a numerical code can be divided into two types of activity: code verification and solution verification (Roache 1998a and b). Solution verification, which may include, for example, tests of convergence of the solution as discretisation in space and time is refined, is carried out on a case-by-case basis by the code user (see the description of quality assurance measures in Appendix C).

In this report, specific code verification exercises are given, together with more detailed code descriptions, in Chapters 3 and 4. Code verification is discussed in these chapters with a focus on numerical algorithm verification. This aims to show that the numerical algorithms in a code are implemented correctly, i.e. consistent with the mathematical formulation of the underlying conceptual model, and that they are functioning as intended. This is achieved, for example, by comparison of results with analytical solutions for simple systems, or with the results of another code.

Code verification of Nagra's safety assessment codes essentially involves two tasks:

- At least at one point in the history of a code, a verification of the treatment of the main processes and a cross-comparison with at least one other, well-established code and / or with analytical solutions is performed.
- Two steps are routinely performed to ensure that each updated version of a code can also be regarded as verified: (i) detailed tests of new capabilities are carried out to check whether these function correctly (e.g. via plausibility checks, comparison with analytical solutions, etc.), and (ii) at least one calculation case, usually a reference case of the preceding major safety assessment, is evaluated with both the old and the new version of the code and a cross-comparison is made. It is only after the updated version of a code has passed steps (i) and (ii) successfully that it may be used in safety assessment.

A further aspect of code verification is software quality engineering (SQE), which aims at showing that a code, as part of a software system, is reliable and produces repeatable results on specific computer hardware and in a specific software environment (Oberkampf & Trucano 2002, 2008). In the dose calculations for SGT Stage 2, this issue is for instance addressed in that the standard verification tests for the codes PICNIC-TD and STMAN, which were originally carried out by the program developer on a specific computer environment to check the proper functioning of these codes, have been successfully rerun using different hardware and a different software environment, which is also the environment used to run the codes in the context of the provisional safety analyses.

3 Models and Codes for the Engineered and Geological Barriers

This chapter describes in detail the conceptual models and the safety assessment codes for radionuclide release and transport in the engineered and geological barriers of the repository systems and highlights their relationships to the relevant processes and parameters in Appendix A. To this end, a description of the underlying generic concepts of radionuclide release and transport in the engineered and geological barriers is given in Section 3.1, followed by a presentation of their mathematical treatment in Section 3.2. The safety assessment codes themselves are described in Sections 3.3 to 3.5.

3.1 Generic concepts of radionuclide release and transport

The generic concepts (or generic conceptual models) of radionuclide release and transport as described in the following paragraphs are specific to the reference release scenario to be investigated in the context of the present dose calculations, i.e. the release of dissolved radionuclides along the groundwater pathway under the premise that the engineered barriers function correctly.

Overall, it is assumed that all materials in the repository near field and the surrounding rock units that may contain / transport radionuclides are porous media. Note that this basic assumption is conceptually also made for water-conducting features in the geosphere without porous infill (e.g. open joints) and for other void volumes, such as the void space inside of a breached disposal canister. Fig. 3-1a shows an illustration of such a porous medium, consisting of an interconnected pore space between solid particles.

In line with Bear & Cheng (2010), water flow and solute transport in the various porous media are conceptualised using continuum models. This concept rests upon the assumption that any heterogeneity at the microscopic level, e.g. with respect to pore flow velocity or solid grain size, can be averaged over a macroscopic representative elementary volume (REV). In the continuum models, both the solid matrix and the void space conceptually coexist at any location within the REV. In the dose calculations for the provisional safety analyses it is further assumed that the pore space of a porous medium is occupied completely by the aqueous phase. The aqueous phase, also termed pore water, may be stagnant or subject to water flow, which is assumed to be governed by Darcy's law.[20]

The nuclide inventory of the radioactive waste is generally assumed to be embedded in one or several homogeneous waste matrices. In the case of LLW, ILW and vitrified HLW (which all result from specific waste conditioning processes[21]), a single waste matrix type is considered. In the case of spent fuel, two types of waste matrix are distinguished:

- the spent fuel matrix, and
- the Zircaloy cladding and other structural elements.

[20] As noted in Kosakowski (2004), Darcy's law gives an upper limit for flow velocities in low-permeable porous media.

[21] Examples for such processes are cementation, bituminisation and vitrification.

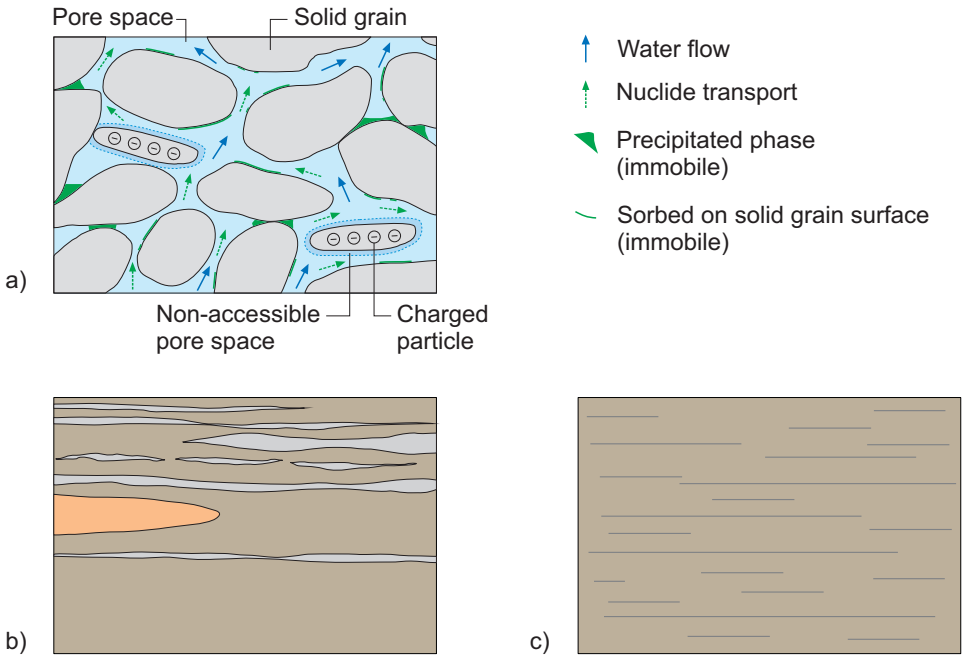

Fig. 3-1: Illustration of solute transport and retardation of a single nuclide in a water-saturated porous medium (a), illustration of a typical rock unit with anisotropic properties (b) and conceptualisation of this rock unit as homogeneous porous medium (HPM) with equivalent anisotropic water flow and solute transport properties (c).

The onset of nuclide release to solution may be delayed by some sort of containment, e.g. a tight disposal canister. Thereafter, depending on the characteristics of the individual waste matrices, a fraction of the nuclide inventory may be released relatively rapidly when in contact with the aqueous phase. For example, in case of the spent fuel matrix, a part of the inventory of some nuclides will have accumulated at fuel grain boundaries, fuel pellet cracks and the gap between the fuel pellets and the cladding. This fraction is thus assumed to be released rather quickly. The remainder of the nuclide inventory is considered to be uniformly distributed in the respective waste matrices and to be released gradually as these corrode or degrade.

Radionuclides are subject to α-, β- or γ-decay before, during and after release from the waste matrices.[22] Once released from the waste matrices, each radionuclide or stable isotope is, in general, considered to behave as an independent substance in the aqueous phase, regardless of whether it is dissolved, in a complex with carbonates and organics or attached to some colloid. In other words, there is generally assumed to be no physicochemical interaction between nuclides. However, nuclides may precipitate as a solid phase if solubility limits of the element, of which they form an isotope, are exceeded (see below).

Nuclides migrate through the pore space by molecular diffusion and, if water flow occurs, by advection. For a given nuclide, the same amount of pore space is generally assumed to be available to all transport processes, although, under certain circumstances, the pore space accessible for diffusive transport is assumed to differ from the pore space available for advective transport. The mathematical approach to deal with this dualism is described in Section 3.2.6.

[22] Other decay modes are considered negligible.

Diffusive transport is assumed to follow Fick's first law. The complex interplay of different diffusion processes (e.g. pore diffusion, surface diffusion) with the pore space geometry (tortuosity, constrictivity) is simplified by using an integrated, element-specific parameter termed effective diffusion coefficient (see van Loon 2012).

If nuclides are transported advectively, the plume is dispersed due to microscopic and macroscopic heterogeneities present in the porous medium and the non-uniform flow pattern therein (mechanical dispersion). This process is conceptualised as a diffusion-like process, also described by Fick's first law. Dispersion in flow direction (longitudinal dispersion) may be different from that perpendicular to flow direction (transverse dispersion), the latter being assumed to be significantly smaller than the former. The sum of mechanical dispersion and diffusion is usually referred to as hydrodynamic dispersion (Bear & Cheng 2010).

Macroscopic heterogeneities may also result in characteristics of the porous medium (e.g. hydraulic conductivity and diffusive transport properties) that are dependent of direction (anisotropy, see b) and c) in Fig. 3-1). This is particularly the case for the geological barrier in most geological siting regions as a result of their sedimentary genesis (e.g. small-scale bedding, macroscopic lenses).

The transport of some nuclides may be retarded by sorption on accessible surfaces of solid particles or on interlayer positions of certain minerals along their migration paths (see Fig. 3-1a). Sorption is pessimistically assumed to be fully reversible. Sorption is further assumed to be linear, which means that the amount sorbed is proportional to the concentration in the pore water. This implies that sorption is sufficiently rapid that an equilibrium can be assumed to exist at any given time between the amount of a nuclide that is sorbed and the amount present in solution (see Nagra 2014b and references therein). Furthermore, the assumption of proportionality between these two quantities is appropriate given that, except within and around the waste forms, radionuclides are generally present in trace amounts. Because, as illustrated in Fig. 3-1, the surface of some particles may be charged, the accessible pore space for nuclides that are similarly charged may be lower than for oppositely charged or neutral nuclides. This phenomenon is called anion exclusion.

A nuclide will precipitate if the concentration of the element of which it is an isotope exceeds its solubility limit. The precipitate redissolves if the element concentration subsequently falls below the solubility limit. To model precipitation and redissolution, it is assumed that the proportions of the isotopes are equal in the aqueous and the precipitated phase. Precipitation and redissolution are most relevant to nuclides that are released from the waste forms in relatively large quantities and / or that are isotopes of other nuclides that are either released in large quantities simultaneously (like U and Pu), or that are already present, typically as stable isotopes, in the pore water (e.g. inorganic carbon in cementitious materials). Because only trace amounts of radionuclides are expected to reach the geosphere, solubility limitation is generally only relevant to near-field release and transport modelling. Co-precipitation, i.e. the immobilisation of a soluble substance in the precipitate of another substance, may in reality also occur in some circumstances. This process is considered negligible and is thus omitted in the generic concepts.

It is important to note that (i) all sorbed and precipitated nuclides are conceptually immobile until desorbed or redissolved, and (ii) sorption and precipitation are assumed to be unselective with respect to the various isotopes of an element. The generic concepts further assume that (iii) sorbed and precipitated nuclides do not affect porosity and (iv) sorption and dissolution / precipitation are in local equilibrium, that is to say the kinetics of these processes are assumed to be rapid compared to the timescales of interest.

Table 3-1 gives an overview of the processes explicitly included in the generic concepts of radionuclide release and transport in the engineered and geological barriers and shows their link to the relevant processes and parameters of Appendix A. This table also shows which processes are implemented in the individual safety assessment codes. Note that there is more than one code that can, in principle, be used to model either the repository near field or the geosphere. Sections 5.3.6 and 5.4.5 explain in detail the selection of specific codes for near-field or geosphere calculations as part of the dose calculations as part of the provisional safety analyses.

Tab. 3-1: Processes explicitly included in the generic concepts of radionuclide release and transport in the engineered and geological barriers.

A complete list of the relevant processes and parameters is given in Appendix A. In this table, only the processes that are addressed explicitly by the codes are mentioned. Sections 5.3.6 and 5.4.5 explain in detail the selection of specific codes for near-field or geosphere calculations.

Process	**Relevant processes and parameters**		**Safety assessment codes**		
	Engineered barriers (near field)	**Geological barriers (geosphere)**	**VPAC**	**STMAN**	**PICNIC-TD**
Radioactive decay and ingrowth			×	×	×
Radionuclide containment	PT-1		×	×	(×) [1]
Release of radionuclides (and stable isotopes) to solution	PT-2		×	×	(×) [1]
Groundwater flow and advective/dispersive transport in solution	PT-5	PG-6, PG-7, PG-8, PG-9, PG-10, PG-13, PG-14	×	×	×
Diffusive transport in solution	PT-5	PG-9, PG-10, PG-13, PG-22	×	×	×
Sorption	PT-4	PG-9, PG-10, PG-21	×	×	×
Precipitation	PT-3		×	×	

[1] In general, near-field release rates are read by PICNIC-TD from a file produced by another code (generally STMAN). However, PICNIC-TD also incorporates a number of simple, analytical release functions.

3.2 Mathematical representation

3.2.1 Initial nuclide inventory within waste forms and its partitioning

Conceptually, a part of the nuclide inventory within a waste form may be assumed to be released relatively rapidly when in contact with the aqueous phase. The proportion of the total inventory represented by this part is termed the instant release fraction (IRF). The respective amount is termed the instant release inventory. For single nuclides, the IRF is, to a good approximation, independent of time, since the material-altering processes that give rise to, and determine the size of, the IRF (e.g. in the wake of reactor operation) have virtually ceased by the time of waste emplacement (see Section 5.3.2). However, in the case of a nuclide that is the progeny of another nuclide within a decay chain, its IRF will change over time, unless the nuclide and its parent have the same IRF values.

In mathematical terms, the total initial inventory $I^N(t_0)$ [M] of a nuclide N in a given waste form at the beginning of the time frame for safety assessment t_0 (in Chapter 5 also called the reference point in time) is subdivided into a total initial instant release inventory $N_{IRF}^N(t_0)$ (which is the sum of the instant release inventories over the individual matrix types m):

$$N_{IRF}^N(t_0) = \sum_m IRF_m^N \cdot I_m^N(t_0) \tag{3.2-1}$$

and one or several gradual release inventories $N_m^N(t_0)$ for each type of waste matrix m:

$$N_m^N(t_0) = (1 - IRF_m^N) \cdot I_m^N(t_0) \tag{3.2-2}$$

with

$I_m^N(t_0)$ total initial inventory of nuclide N in matrix type m [M]

IRF_m^N initial instant release fraction of radionuclide N in matrix type m [-].

Recall that two types of matrix are distinguished for SF, whereas the remaining waste types are assumed to consist of a single waste matrix type.

3.2.2 Radioactive decay within waste forms

During the period of complete containment – and, for the gradual release fractions, also beyond this period – the initial nuclide inventories $N_{IRF}^N(t_0)$ and $N_m^N(t_0)$ are altered by radioactive decay and ingrowth according to:

$$\frac{dN_{IRF}^N(t)}{dt} = -\lambda^N N_{IRF}^N(t) + \sum_B \sigma^{BN}\lambda^B N_{IRF}^B(t) \tag{3.2-3}$$

$$\frac{dN_m^N(t)}{dt} = -\lambda^N N_m^N(t) + \sum_B \sigma^{BN}\lambda^B N_m^B(t) \tag{3.2-4}$$

with

σ^{BN} branching ratio for the decay of parent B into daughter N [-]

λ^N decay constant of nuclide N [1/T][23]

λ^B decay constant of parent radionuclide B [1/T].

As pointed out in the previous section, the resulting IRFs for decay chain members can vary with time. However, this is not relevant in the context of the provisional safety analyses, since only single nuclides are attributed IRFs.

Processes leading to loss of containment are not explicitly modelled. Rather, the assumption made is that loss of containment occurs instantaneously and completely at a given time. For example, it is assumed that, once the disposal canisters for SF and HLW have been breached at time t_c, they no longer prevent water ingress or nuclide release. Any internal types of containment, e.g. the HLW fabrication flasks, are also taken to be lost by the time that the disposal canisters are breached.

The duration of the period of complete containment is an input parameter to the codes addressing near-field release and transport (VPAC and STMAN) and refers to the relevant parameter PT-1 (see Appendix A).

3.2.3 Release to solution

At the end of the period of complete containment at time t_c, water is assumed to come into contact with the waste forms and the instant release inventory $N_{IRF}^N(t_c)$ is instantaneously released to solution. The waste forms start to slowly dissolve or corrode, thus gradually releasing the remaining inventory (see below). The total nuclide release rate $G^N(t)$ [M T^{-1}] is given by:

$$G^N(t) = N_{IRF}^N(t) \cdot \delta(t - t_c) + \sum_m N_m^N(t) \cdot f_m(t) \qquad (3.2\text{-}5)$$

with

δ Dirac's delta-function [T^{-1}]

t_c time of loss of containment [T]

$f_m(t)$ fractional release rate from matrix type m as a function of time t [T^{-1}].

Note that $N_m^N(t)$ is subject to continuous radioactive decay and ingrowth following eq. 3.2-4.

The fractional release rate is defined as:

$$f_m(t) = \frac{1}{V_m(t_c)} \cdot \frac{dV_m(t)}{dt} \qquad (3.2\text{-}6)$$

with

$V_m(t)$ volume of unaltered or uncorroded matrix type m, as a function of time t [L^3].

---

[23] This value is zero for stable nuclides.

It is further assumed that the volume of matrix type m does not change during the period of complete containment, i.e. $V_m(t_c) = V_m(t_0)$. The fractional release rates $f_m(t)$ refer to the relevant parameter PT-2 (see Appendix A).

The equation 3.2-6 is based on the assumption of congruent release. This means that nuclides are released at the same rate as the unaltered or uncorroded matrix volume decreases with time, implying uniform distribution of the nuclides in the matrix (and also, conservatively, that alteration or corrosion products do not take up any nuclides). The rate at which the volume of the unaltered or uncorroded waste matrix changes is proportional to a dissolution / corrosion rate k [L T^{-1}]. This rate k is equal to the specific corrosion or dissolution rate r [M L^{-2} T^{-1}] divided by the density of the waste matrix ρ [M L^{-3}]). The rate of volume change is also proportional to the wetted surface area of the matrix [L^2], which may itself be a function of time t. The wetted surface area depends on the external geometry of the waste matrix and also on any fracturing that allows water to access its internal surfaces.

Fig. 3-2 shows an example of the total amount of a nuclide released as a function of time, considering initial containment, an instant release fraction and congruent release at a constant rate. For illustrative purposes, the case of a stable nuclide without any progeny is presented.

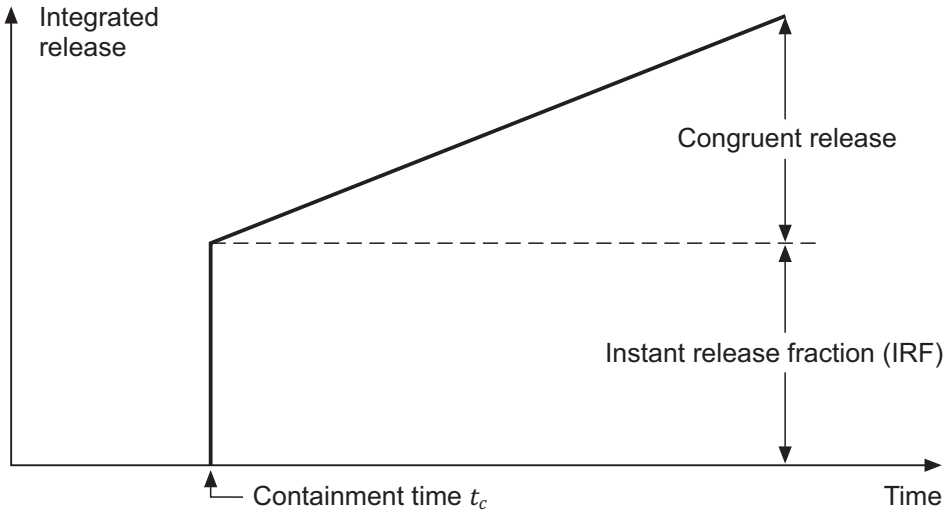

Fig. 3-2: Example of total amount of a stable nuclide without parent nuclide released as a function of time.

The example considers initial containment, an instant release fraction and congruent release with corrosion (or dissolution) at a constant rate. Note also that the curve considers one matrix type only.

In the case of vitrified high-level waste (HLW), the specific glass dissolution rate (i.e. the dissolution rate per unit surface area of wetted glass r, sometimes simply called the glass corrosion rate) is assumed to be constant (see Section 5.3.2). However, fracturing of the glass is assumed to have taken place during cooling, so that the wetted surface area is higher than the external area of an unfractured glass block. In the following, a simple model is developed, in which the glass fragments are represented conceptually as a number of spheres of equal size. Although this model is rather specific, it is reported in this chapter, since it is directly implemented in the

STMAN code, which is also described later in this chapter. Furthermore, it is sufficiently generic to allow any total dissolution time to be modelled[24].

The radius of the spheres r_s [L] is fixed by the condition that the initial ratio of glass volume to surface area is the same for the spheres as for the real fractured glass block:

$$r_s = \frac{3 \cdot V_0}{A_0} \tag{3.2-7}$$

V_0 initial total volume of the block [L^3]

A_0 initial total surface area [L^2].

The number of spheres n_s is fixed by the further condition that the total volume of the spheres is equal to the total volume of the block:

$$n_s = \frac{3 \cdot V_0}{4 \cdot \pi \cdot r_s^3} \tag{3.2-8}$$

The assumption of a constant glass-corrosion rate per unit surface area leads to a rate of decrease in the radius of the spheres that is proportional to time, so that the lifetime of the spheres is given by τ [T]:

$$\tau = \frac{\rho \cdot r_s}{r} = \frac{3 \cdot \rho \cdot V_0}{r \cdot A_0} \tag{3.2-9}$$

The fractional release rates then becomes:

$$f_{\mathrm{HLW}}(t) = \begin{cases} \frac{3}{\tau}\left(1 - \frac{t - t_c}{\tau}\right)^2, & t_c \le t \le t_c + \tau \\ 0, & \text{else} \end{cases} \tag{3.2-10}$$

3.2.4 Mixing in the interior of a disposal canister and release to the surrounding buffer medium

Consider a nuclide, denoted as isotope N of the chemical element E, which is mobile in the water-filled void space of a breached cylindrical disposal canister (e.g. a disposal canister for SF). The water-filled void space is also termed the reservoir and is, for mathematical convenience, conceptualised as a thin, annular water film at the interface between the disposal canister and the surrounding buffer medium.

[24] The final result (eq. 3.2-10) also applies to any other set of shapes for which the total surface area is proportional to the total volume to the power of 2/3.

Assuming well-mixed conditions, the evolution of the concentration of nuclide N in the reservoir is described by:

$$\frac{\partial\left(\varepsilon^E \cdot R^E \cdot c_l^{N,E}\right)}{\partial t} = \varepsilon^E \cdot DP^{N,E} - \gamma_l^{N,E} + \Theta^N - Y^N \tag{3.2-11}$$

with

$c_l^{N,E}$ concentration in the aqueous phase [M L^{-3}]

ε^E element-specific porosity [-]

$DP^{N,E}$ rate of dissolution / precipitation of nuclide N per unit volume of solution [M L^{-3} T^{-1}], as defined in Section 3.2.9

$\gamma_l^{N,E}$ rate of radioactive decay and ingrowth of nuclide N per unit volume of solution [M L^{-3} T^{-1}]

Θ^N nuclide source term per unit volume of solution [M L^{-3} T^{-1}]

Y^N sink term representing the release of nuclide N to the surrounding buffer medium per unit volume of solution [M L^{-3} T^{-1}]

R^E retardation coefficient for element E [-], which is related to the distribution of the nuclide between the aqueous and sorbed phases and which is defined in Section 3.2.8.

The void space inside a disposal canister is considered a porous medium with negligible amount of solid matrix. Thus, its porosity ε^E and its retardation coefficient R^E are set to unity. However, in the following, these parameters are included explicitly, such that the equations are also applicable to real porous media.

If nuclide N is the progeny of one or several parent nuclides, its rate of radioactive decay and ingrowth $\gamma_l^{N,E}$ is given by:

$$\gamma_l^{N,E} = R^E \cdot \varepsilon^E \cdot \lambda^N \cdot c_l^{N,E} - \sum_{\tilde{E}} \sum_{B} R^{\tilde{E}} \cdot \varepsilon^{\tilde{E}} \cdot \sigma^{BN} \cdot \lambda^B \cdot c_l^{B,\tilde{E}} \tag{3.2-12}$$

where the outer summation is taken over all chemical elements and the inner summation is taken over the isotopes B of element $\tilde{E}$ that are parents of nuclide N (only elements with one or more isotopes that are parents of N contribute to the outer summation).

Θ^N, the nuclide source term, is given by:

$$\Theta^N = \frac{G^N(t)}{V_R} \tag{3.2-13}$$

where V_R is the volume of the reservoir [L^3].

Based on the assumptions of a fully breached disposal canister and radial diffusion being the only significant solute transport process to the surrounding porous buffer medium BM, the sink term is written as:

$$Y^N = -2\pi \cdot r_0 \cdot L_c \cdot \left(\varepsilon_{BM}^E \cdot D_{p,BM}^E \cdot \frac{\partial c_{BM,l}^{N,E}}{\partial r} \right)\Bigg|_{r=r_0} \tag{3.2-14}$$

with

$c_{BM,l}^{N,E}$ nuclide concentration in the pore water of the surrounding buffer medium [M L^{-3}]

r radial distance from the canister axis [L]

r_0 radius of disposal canister [L]

L_c length of disposal canister [L]

ε_{BM}^E element-specific porosity in the surrounding buffer medium BM [-]

$D_{p,BM}^E$ pore diffusion coefficient of element E in the surrounding buffer medium BM [L^2 T^{-1}].

and the boundary condition:

$$c_{BM,l}^{N,E}\big|_{r=r_0} = c_l^{N,E}. \tag{3.2-15}$$

If the solubility limit of element E is reached, the nuclide is also present as a solid precipitate. The evolution of the concentration of the precipitate is described by:[25]

$$\frac{\partial\left(\varepsilon^E \cdot c_s^{N,E}\right)}{\partial t} = -\varepsilon^E \cdot DP^{N,E} - \gamma_s^{N,E} \tag{3.2-16}$$

with

$c_s^{N,E}$ concentration of the precipitate [M L^{-3}]

$DP^{N,E}$ rate of dissolution / precipitation of nuclide N per unit volume of solution [M L^{-3} T^{-1})], as defined in Section 3.2.9

$\gamma_s^{N,E}$ rate of radioactive decay and ingrowth of nuclide N in the precipitate per unit volume of solution [M L^{-3} T^{-1}].

The rate of radioactive decay and ingrowth $\gamma_s^{N,E}$ in the precipitate is given by:

$$\gamma_s^{N,E} = \varepsilon^E \cdot \lambda^N \cdot c_s^{N,E} - \sum_{\tilde{E}} \sum_{B} \varepsilon^{\tilde{E}} \cdot \sigma^{BN} \cdot \lambda^B \cdot c_s^{B,\tilde{E}} \tag{3.2-17}$$

No sink term to the surrounding buffer medium is provided in equation 3.2-16, as solid precipitates are assumed to be not able to penetrate into this medium.

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[25] Note that in the VPAC code, it is conceptually assumed that the concentration of the precipitate refers to the volume of the solid matrix $(1 - \varepsilon^E)$. This assumption is, however, of no consequence for the calculated results.

3.2.5 Water flow

The rate of water flow in the various porous media is generally assumed to follow Darcy's law[26]:

$$\vec{q} = -K \cdot \nabla h, \text{ or } \vec{q} = -K \cdot \vec{\imath} \tag{3.2-18}$$

with

$\vec{q}$ Darcy velocity [L T^{-1}]

h hydraulic head [L]

K hydraulic conductivity [L T^{-1}]

$\vec{\imath}$ hydraulic gradient [L L^{-1}].

The porous medium may show some anisotropy with respect to hydraulic conductivity, e.g. as a result of the layered structure of a sedimentary rock. In the dose calculations for the provisional safety analyses, bedding in the ECZ is assumed to be horizontal (see Chapter 5), in which case the hydraulic conductivity is written as a symmetric tensor $\boldsymbol{K}$ [L T^{-1}] with zero off-diagonal terms:

$$\boldsymbol{K} = \begin{bmatrix} K_h & 0 & 0 \\ 0 & K_h & 0 \\ 0 & 0 & K_v \end{bmatrix} \tag{3.2-19}$$

and with

K_h horizontal hydraulic conductivity (parallel to bedding) [L T^{-1}]

K_v vertical hydraulic conductivity (orthogonal to bedding) [L T^{-1}].

The hydraulic head is linked to the pressure field of the aqueous phase via the equation:

$$h = \frac{p}{\rho \cdot g} + z \tag{3.2-20}$$

with

p pressure in aqueous phase [M L^{-1} T^{-2}]

z elevation above reference level [L]

ρ fluid density [M L^{-3}]

g gravitational acceleration [L T^{-2}].

[26] In particular, it is assumed that no threshold gradient exists.

Finally, the continuity equation for groundwater flow is as follows:

$$S_s \frac{\partial h}{\partial t} + \nabla \cdot \vec{q} = f \tag{3.2-21}$$

with

S_s specific storage coefficient [L^{-1}]

f hydraulic source term [T^{-1}].

The hydraulic conductivity and the hydraulic gradient both refer to the relevant near-field parameter PT-5 as well as to the relevant geosphere parameters PG-6, PG-7 and PG-8 (see Appendix A). The specific storage coefficient is not considered to be a relevant parameter, as any change in the liquid pressure field is expected to occur rapidly in comparison with geological time scales (see Section 5.2).

3.2.6 General equation for solute transport

Consider again a nuclide, denoted as isotope N of the chemical element E. Assume that the nuclide is mobile in solution, sorbed onto particle surfaces or precipitated. Transport of the nuclide in the aqueous phase is then described in a very general form by:

$$\begin{aligned}\frac{\partial\left(\varepsilon^E \cdot R^E \cdot c_l^{N,E}\right)}{\partial t} + \nabla \cdot \left(\vec{q} \cdot c_l^{N,E}\right) - \nabla \cdot \left(\varepsilon^E \cdot \boldsymbol{D^E} \cdot \nabla c_l^{N,E}\right) \\ = \varepsilon^E \cdot DP^{N,E} - \gamma_l^{N,E} + \Theta^N\end{aligned} \tag{3.2-22a}$$

If one considers a one-dimensional transport path (let us say in direction of the x-coordinate), along which the Darcy velocity $\vec{q}$ and other transport properties are assumed not to vary, then eq. 3.2-22a simplifies to:

$$R^E \cdot \varepsilon^E \cdot \frac{\partial c_l^{N,E}}{\partial t} = \varepsilon^E \cdot D^E \cdot \frac{\partial^2 c_l^{N,E}}{\partial x^2} - q \cdot \frac{\partial c_l^{N,E}}{\partial x} + \varepsilon^E \cdot DP^{N,E} - \gamma_l^{N,E} + \Theta^N \tag{3.2-22b}$$

In the above equation the dispersion / diffusion tensor $\boldsymbol{D^E}$, described below, reduces to a scalar quantity D^E [L^2 T^{-1}] that describes diffusion and longitudinal dispersion along the transport path.

Θ^N, the nuclide source term, is given by:

$$\Theta^N = \begin{cases} \dfrac{G^N(t)}{V_m}, \text{ in a region occupied by waste form } m \text{ with volume } V_m \\ 0, \text{ elsewhere} \end{cases} \tag{3.2-23}$$

Note that, in the case of waste inside of a disposal canister, the region occupied by the waste form lies outside the domain in which nuclide transport is modelled explicitly. The mathematical description of nuclide release in this region is described in Section 3.2.4.

The tensor $\boldsymbol{D}^E$ describes the combined effect of mechanical dispersion and pore diffusion (hydrodynamic dispersion):

$$\boldsymbol{D}^E = \begin{bmatrix} D_{xx} & D_{yx} & D_{zx} \\ D_{xy} & D_{yy} & D_{zy} \\ D_{xz} & D_{yz} & D_{zz} \end{bmatrix} + D_p^E \cdot \boldsymbol{I} \tag{3.2-24}$$

D_p^E isotropic pore diffusion coefficient for element E [L^2 T^{-1}]

$\boldsymbol{I}$ unit tensor [-]

The elements of the mechanical dispersion tensor in eq. 3.2-24 are expressed as:

$$D_{ij} = \alpha_T \cdot \left|\overrightarrow{u^E}\right| \cdot \delta_{ij} + (\alpha_L - \alpha_T) \cdot \frac{u_i^E \cdot u_j^E}{\left|\overrightarrow{u^E}\right|} \tag{3.2-25}$$

with

$\delta_{ij} = 1$ if $i = j, \delta_{ij} = 0$ if $i \neq j$ [-]

α_L longitudinal dispersion length [L]

α_T transverse dispersion length [L]

$\overrightarrow{u^E}$ average linear velocity of element E [L T^{-1}]

u_i^E component of average linear velocity along the i-axis [L T^{-1}].

The average linear velocity of element E is related to the Darcy velocity as follows:

$$\overrightarrow{u^E} = \frac{\vec{q}}{\varepsilon^E} \tag{3.2-26}$$

If the porous medium shows anisotropic behaviour with respect to dispersion and if this anisotropy is aligned with the considered coordinate system, then the mechanical dispersion tensor may be written as a symmetric tensor. If the same is true for diffusion, then $D_p^E \cdot \boldsymbol{I}$ in eq. 3.2-24 is replaced by the diagonal matrix $\boldsymbol{D}_p^E$ [L^2 T^{-1}]:

$$\boldsymbol{D}_p^E = \begin{bmatrix} D_{p,h}^E & 0 & 0 \\ 0 & D_{p,h}^E & 0 \\ 0 & 0 & D_{p,v}^E \end{bmatrix} \tag{3.2-27}$$

with

$D_{p,h}^E$ horizontal pore diffusion coefficient for element E (parallel to bedding) [L^2 T^{-1}]

$D_{p,v}^E$ vertical pore diffusion coefficient for element E (orthogonal to bedding) [L^2 T^{-1}].

In Section 3.1, it is pointed out that the process of diffusion is described by a single integrated element-specific parameter termed effective diffusion coefficient. In the transport equations above, this quantity is reformulated as the product of the element-specific porosity and a pore diffusion coefficient, which then integrates all the other characteristics of the diffusion process. This is how diffusion is modelled in the VPAC code. In contrast, with STMAN and PICNIC-TD, the effective diffusion coefficient is used directly.

For some porous media, the element-specific porosity values relevant to advection of a nuclide may be different from those relevant to its diffusion. Since VPAC only allows a single porosity value, the element-specific porosity ε^{E}, to be defined for each nuclide in the input file of a given VPAC model denotes the porosity accessible for advective transport and the VPAC input parameter pore diffusion coefficient is scaled such that the product $\varepsilon^{E} \cdot D^{E}_{p,scaled}$ yields the desired effective diffusion coefficient.

If the nuclide is also present as a solid precipitate, the evolution of the concentration of the precipitated phase is given by an equation analogous to eq. 3.2-16.

In the case of the geological barriers, the element-specific porosity is related to the relevant parameter PG-10 (see Appendix A). The pore diffusion coefficient is associated with the parameters PT-5 and PG-22. Transport path lengths are derived from the dimensions of the modelled porous medium and, in the case of the geological barriers, are related to the relevant parameter PG-13.

3.2.7 Solute transport along discrete water-conducting features

Discrete water-conducting features in a rock, such as faults and joints[27], may be conceptualised as zones occupied by homogeneous porous media, as defined in Section 3.1. If transport in the rock matrix is assumed to be negligible, the equations for solute transport from Section 3.2.6 apply. There is, however, an alternative conceptualisation that considers solute transport in the water-conducting features and in the rock matrix as separate but coupled processes. This alternative conceptualisation is frequently used for modelling nuclide transport along discrete water-conducting features in the geosphere.[28]

Fig. 3-3 illustrates the case where the water-conducting feature is a narrow, planar fracture of aperture $2b$. Both the fracture and the rock matrix conduct water in the x-direction. The fracture aperture is assumed to be sufficiently small that the nuclide concentration in the water flowing through the fracture can be assumed to be uniform in the z-direction. Nuclides can be transferred between the fracture and the rock matrix by diffusion in z-direction. It is assumed that the extent of the accessible rock matrix is limited to a distance $(B - b)$ from the fracture / matrix interface, i.e. to a distance B from the fracture centre line.

[27] In this report, the terms fracture and transmissive element are both used as umbrella terms for discontinuities such as faults and joints.

[28] In the literature, this is also known as double-porosity or dual-porosity approach.

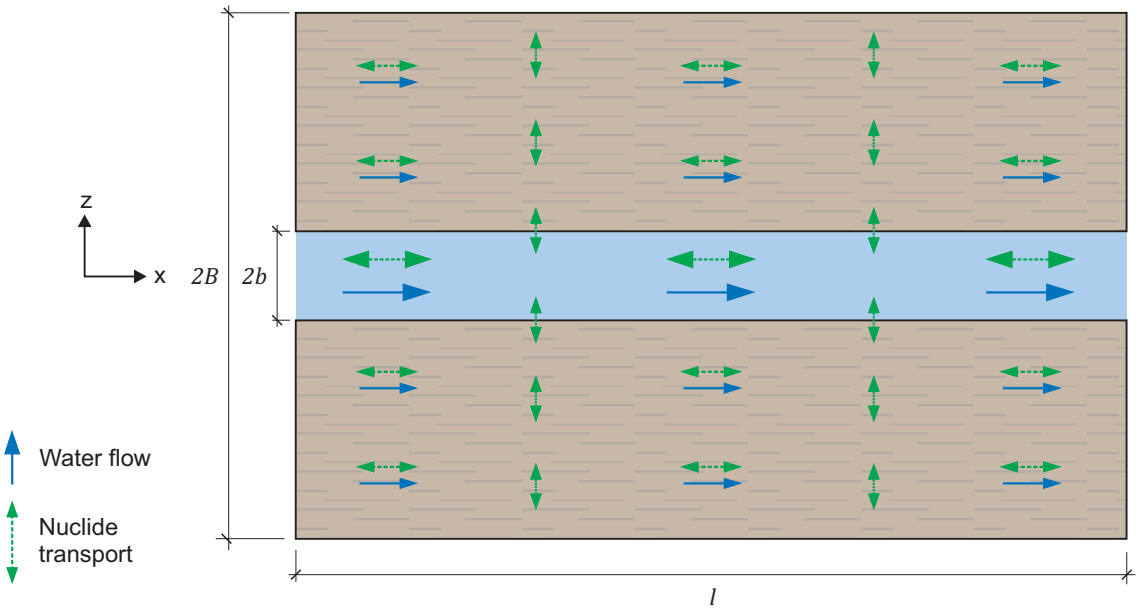

Fig. 3-3: Alternative concept of solute transport along discrete water-conducting features.

In the absence of any nuclide source and disregarding any precipitation / dissolution reactions, transport in the rock matrix is described by a simplified form of eq. 3.2-22a:[29]

$$\frac{\partial(\varepsilon^E \cdot R^E \cdot c^{N,E})}{\partial t} + \frac{\partial}{\partial x}\left(q \cdot c^{N,E}\right) - \nabla \cdot (\varepsilon^E \cdot \boldsymbol{D^E} \cdot \nabla c^{N,E}) = -\gamma^{N,E} \qquad (3.2\text{-}28)$$

with

$c^{N,E}$ concentration of nuclide N of chemical element E in the rock matrix [M L^{-3}]

q Darcy velocity in the rock matrix [M L^{-1}].

Transport in the fracture is described by:

$$\frac{\partial(\varepsilon_L^E \cdot R_L^E \cdot P^{N,E})}{\partial t} + \frac{\partial}{\partial x}\left(q_L \cdot P^{N,E}\right) - \frac{\partial}{\partial x}\left(\varepsilon_L^E \cdot D_L^E \cdot \frac{\partial P^{N,E}}{\partial x}\right) = -\gamma_L^{N,E} - \Theta^N \qquad (3.2\text{-}29)$$

with

$P^{N,E}$ concentration of nuclide N of chemical element E in the pore space of the fracture [M L^{-3}]

ε_L^E element-specific porosity of the fracture interior [-]

q_L Darcy velocity in the fracture [L T^{-1}]

R_L^E retardation coefficient of element E due to sorption on fracture surfaces or infill [-]

[29] Note that, in the PICNIC code, radionuclide concentrations and the properties of the matrix are assumed not to vary along y, such that the ∇-operator is only applied in the x-z plane. Note further that transverse dispersion in the rock matrix is not considered in this approach.

$\gamma_L^{N,E}$ rate of radioactive decay and ingrowth of nuclide N per unit volume of solution in the fracture [M L^{-3} T^{-1}]

Θ^N sink term (see below) [M L^{-3} T^{-1}] .

If the nuclide N is the progeny of one or several parent nuclides, its rate of radioactive decay and ingrowth $\gamma_L^{N,E}$ in the fracture is given by:

$$\gamma_L^{N,E} = R_L^E \cdot \varepsilon_L^E \cdot \lambda^N \cdot P^{N,E} - \sum_{\tilde{E}} \sum_{B} R_L^{\tilde{E}} \cdot \varepsilon_L^{\tilde{E}} \cdot \sigma^{BN} \cdot \lambda^B \cdot P^{B,\tilde{E}} \tag{3.2-30}$$

where the outer summation is taken over all chemical elements and the inner summation is taken over the isotopes B of element $\tilde{E}$ that are parents of nuclide N (only elements with one or more isotopes that are parents of N contribute to the outer summation).

In eq. 3.2-29, a sink term is introduced that describes diffusive transfer to the adjoining rock matrix:

$$\Theta^N = -\varepsilon_L^E \cdot \delta_L \cdot \left(\varepsilon^E \cdot D_z^E \cdot \frac{\partial c^{N,E}}{\partial z} \right)\Big|_{z=b} \tag{3.2-31}$$

with the boundary condition:

$$c^{N,E}\big|_{z=b} = P^{N,E} \tag{3.2-32}$$

and

δ_L surface area of the rock matrix per unit volume of flowing water in the fracture [L^{-1}]

D_z^E pore diffusion coefficient in the matrix in z-direction [L^2 T^{-1}].

In the case of a narrow planar fracture as illustrated in Fig. 3-3:

$$\delta_L = \frac{1}{b \cdot \varepsilon_L^E} \tag{3.2-33}$$

D_L^E accounts for the combined effects of diffusion and mechanical dispersion in the fracture in the longitudinal (flow) direction:

$$D_L^E = \frac{\alpha_L \cdot q_L}{\varepsilon_L^E} + D_{p,L}^E \tag{3.2-34}$$

with

$D_{p,L}^E$ pore diffusion coefficient of element E in the fracture [L^2 T^{-1}].

The longitudinal dispersion length can be written in terms of a Peclet number Pe:

$$\alpha_L = \frac{l}{Pe} \tag{3.2-35}$$

with

l length of the fracture in flow direction [L].

The flow velocity in a discrete water-conducting feature is usually calculated from the transmissivity of the feature T [L^2 T^{-1}]:

$$q_L = \frac{T}{2 \cdot b} \cdot i \tag{3.2-36}$$

with

i hydraulic gradient in flow direction [L L^{-1}].

The length of the fracture in flow direction l is related to the relevant parameter PG-13 (see Appendix A). The transmissivity T refers to the parameters PG-14 and PG-8, if solute transport in a single discrete feature is modelled, and to the parameters PG-6, PG-7, PG-8 and PG-9, if a group of water-conducting features show a regular and frequent pattern that uniformly affects the large-scale hydraulic conductivity of the rock unit under consideration. In the latter case, the transmissivity is related to the equivalent hydraulic conductivity of the rock unit in flow direction, $K_{\text{equivalent}}$ [L T^{-1}], and to the hydraulic conductivity of the rock matrix, $K_{\text{rock matrix}}$ [L T^{-1}], by:

$$\frac{T}{2 \cdot B} = K_{\text{equivalent}} - \left(\frac{B-b}{B}\right) K_{\text{rock matrix}} \approx K_{\text{equivalent}} - K_{\text{rock matrix}} \tag{3.2-37}$$

assuming, as is normally the case, that the fracture aperture is small compared with fracture spacing.

3.2.8 Sorption and retardation

Based on the assumption of linear, equilibrium sorption of nuclides along the migration path, the retardation coefficient R^E of element E in a porous medium is given by:

$$R^E = 1 + \frac{K_d^E \cdot \rho_s}{\varepsilon^E} \tag{3.2-38}$$

with

K_d^E sorption coefficient of element E [L^3 M^{-1}]

ρ_s dry bulk density [M L^{-3}].

For some materials, it is more convenient to rewrite this expression in terms of the (average) density of the component mineral grains ρ_{grain} [M L^{-3}]:

$$R^E = 1 + \frac{K_d^E \cdot (1-\varepsilon) \cdot \rho_{\text{grain}}}{\varepsilon^E} \tag{3.2-39}$$

where ε is the total porosity.

The sorption coefficients are related to the relevant parameters PT-4 and PG-21 (see Appendix A).

3.2.9 Precipitation and dissolution

A nuclide may precipitate if the concentration of the element of which it is an isotope exceeds its solubility limit. Furthermore, it will redissolve if the element concentration subsequently falls below the solubility limit. Concentrations of all isotopes of element E, including, if required, any stable isotopes, are taken into account when evaluating whether the solubility limit of element E has been reached. Specifically, the maximum possible concentration of all isotopes of an element E is set equal to the elemental solubility limit c_{sol}^E [M L^{-3}].

The maximum possible concentration of a specific isotope N, $c_{\text{sol}}^{N,E}$ [M L^{-3}], is obtained by scaling c_{sol}^E by the ratio of the aqueous concentration of nuclide N to the total aqueous concentration of all isotopes i of the corresponding element E. In other words, the scaling is such that the proportions of the isotopes are equal in both the aqueous phase and the precipitated phase:

$$c_{\text{sol}}^{N,E} = c_{\text{sol}}^E \cdot \frac{R^E \cdot c_l^{N,E} + c_s^{N,E}}{\sum_i \left[R^E \cdot c_l^{i,E} + c_s^{i,E}\right]} \tag{3.2-40}$$

It is generally assumed that precipitation and dissolution take place very quickly, such that the following criteria are satisfied:

$$\left[c_s^{N,E} = 0 \text{ and } c_l^{N,E} \le c_{\text{sol}}^{N,E}\right] \text{ or } \left[c_s^{N,E} > 0 \text{ and } c_l^{N,E} = c_{\text{sol}}^{N,E}\right] \tag{3.2-41}$$

The value of $DP^{N,E}$, i.e. the rate of dissolution (if positive) or precipitation (if negative) appearing in the transport equations of the previous sections, is fixed according to these criteria (see Section 3.3.4 for a description of how this is implemented in VPAC).

The elemental solubility limits c_{sol}^E are related to the relevant parameter of the near field PT-3 (see Appendix A). There is no relation to any relevant parameter of the geological barriers, as the process of precipitation is conservatively omitted in the geosphere (see Section 5.4).

3.3 The VPAC code

3.3.1 Scope and purpose

VPAC, or ***V**ersatile **P**erformance **A**ssessment **C**ode*, is an integrated computer code that simulates groundwater flow and nuclide release and transport in a saturated, heterogeneous 2D or 3D porous medium. The porous medium may represent the repository near field, the surrounding geosphere, or both. Discrete water-conducting features (fractures) need to be modelled explicitly as homogeneous porous media.

VPAC is, in principle, suitable for calculating nuclide release and transport for all barrier systems considered in SGT Stage 2. Its strength lies in its ability to model complicated geometrical settings, but at the cost of the separate preparation of a (detailed) numerical mesh and of comparatively long model run times. For rather simple water flow and solute transport problems, the use of VPAC may not be the best choice (see Section 5.3.6).

The general features of the code are documented in detail in a Nagra working report (Holocher et al. 2008), on which the following sections are largely based.

3.3.2 The model domain

The 2D or 3D VPAC model domain can include any spatially distinct feature of the engineered barriers or the geological barrier. All these features are conceptualised as homogeneous porous media and their properties are specified through so-called material classes.

3.3.3 Processes and parameters

The processes represented explicitly in VPAC are:

- saturated groundwater flow, where the hydraulic conductivity may be time dependent;
- release of nuclides (radionuclides and stable isotopes) from the waste matrix, which may be a specified function of time (see below);
- radioactive decay and ingrowth, with an unlimited number of radionuclides and unlimited decay chain lengths;
- advection, dispersion and diffusion of nuclides, with diffusion coefficients that can be time dependent;
- nuclide-specific linear sorption equilibrium between liquid and solid phase, with sorption coefficients that can be time dependent; and
- element-specific solubility limitation.

Nuclides are released either instantaneously and / or gradually, in a time-dependent manner, to the model domain. Optionally, a containment time prior to release can be specified. The time-dependent nuclide release occurs congruently with dissolution or corrosion of the waste matrix. Dissolution / corrosion is calculated from a user-specified rate, and with a user-specified geometry of the waste matrix. Possible geometries are slab geometry, cylinder geometry or spherical geometry.

3.3.4 Solution method

In VPAC, time is discretised into a series of steps. Two calculations are carried out at each time step: a flow calculation and a transport calculation using the flow field obtained in the flow calculations. Hence, the accuracy of the calculated flow field is vital to the accuracy of the transport calculation results.

The Mixed-Hybrid Finite Element Method (MHFEM, see Chavent & Roberts 1991 and Neunhäuserer 2003) is used to solve the flow and transport equation systems at each time step. MHFEM is well suited to the types of model systems to which VPAC is applied, as it allows the exact calculation of nuclide fluxes across arbitrary finite element boundaries. This feature is a necessary requirement for modelling flow and solute transport in complicated geological environments, in which large contrasts in hydraulic and solute transport properties between finite elements may occur.

Each finite element is assigned to a material class. Every material class has its own flow and transport properties, its own initial nuclide inventory (if any) and its own source terms for water and nuclides.

To model the solubility limitation of a dissolved nuclide, the rate of dissolution or precipitation is modelled as follows:

$$DP^{N,E} = \begin{cases} -\sigma \cdot \left(c_l^{N,E} - c_{\mathrm{sol}}^{N,E}\right), \text{ if } \left[c_{\mathrm{sol}}^{N,E} < c_l^{N,E} \text{ or } c_s^{N,E} > 0\right] \\ 0, \text{ if } \left[c_{\mathrm{sol}}^{N,E} > c_l^{N,E} \text{ and } c_s^{N,E} = 0\right] \end{cases} \tag{3.3-1}$$

The numerical parameter σ is set to a constant value that is both positive and sufficiently high to ensure that the criteria given in eq. 3.2-41 are satisfied to a good approximation.

3.3.5 Input requirements

Input data are usually given in plain text files, which need to respect a code-specific XML-file structure. The files are organised hierarchically. Binary files (e.g. the FE mesh) can also be read. Attention has to be paid that all input parameters are given in the units required by the code. The input parameters of VPAC and their default units are summarised in Tab. 3-2.

Flow parameters characterise the hydraulic properties of each material class. The material classes may thus be associated with different hydraulic units. Transport parameters such as sorption coefficients, diffusion coefficients and solubility limits usually vary among different chemical elements. Therefore, these parameters are defined individually for each element and each material class. Nuclide-specific data, such as half-lives, are specified for each nuclide.

The input parameters hydraulic conductivity, pore diffusion coefficient and sorption coefficient may be given values that evolve with time. For each of these time-dependent parameters, the user can create a plain text file, called property time factor file, which contains a list of time points and the corresponding time factor values. The time factor values are then used as multipliers for the initial values.

Usually, only a few pairs of points in time and multipliers (time factors) are provided in a property time factor file. Between these points in time, the time steps and multipliers are interpolated linearly by the code to obtain the multiplier for any required time. This means that, if the hydraulic conductivity is time-dependent and if the value of the hydraulic conductivity changes between two consecutive time steps for at least one material class, the flow field is recalculated at each of these time steps.

Tab. 3-2: VPAC input parameters and default units.

Parameter	Symbol	Default unit	Material-specific	Element- (E) or nuclide-specific (N)	Time-dependent
Water flow and solute transport parameters					
Hydraulic conductivity	$\boldsymbol{K}$	m/s	✓		✓
Specific storage coefficient	S_s	1/m	✓		
Total porosity	ε	-	✓		
Porosity factor	$n^E = \frac{\varepsilon^E}{\varepsilon}$	-	✓	E	
Dispersion lengths	α_L, α_T	m	✓		
Dry bulk density	ρ_s	kg/m^3	✓		
Sorption coefficient	K_d^E	m^3/kg	✓	E	✓
Pore diffusion coefficient tensor	$\boldsymbol{D}_p^E$	m^2/s	✓	E	✓
Solubility limit	c_{sol}^E	mol/m^3	✓	E	
Nuclide and inventory data					
Radionuclide half-life	$T_{1/2} = \frac{\ln 2}{\lambda^N}$	a		N	
Branching ratio	σ^{BN}	-		N	
Instant release fraction	IRF^N	-	✓	N	
Total initial inventory	I^N	mol	✓	N	
Containment time	t_c	a	✓		
Waste geometry model (slab, cylinder or geometry)			✓		
Characteristic size of waste matrix or fragments thereof	r_s	m	✓		
Corrosion / dissolution rate	k	m/s	✓		

3.3.6 Verification

Verification of VPAC 1.1 includes:

- individual verification of the treatment of the main processes and their implementation in the earlier code version VPAC 1.0,
- benchmark exercises for the earlier code version VPAC 1.0 using the AMBER code (Quintessa 2010) and also analytical solutions that address the full set of included processes,
- the recalculation of selected calculation cases from the latest officially approved safety assessment, as reported in Nagra (2010a), and
- a detailed test of the new anisotropic diffusion capability in VPAC 1.1 and an investigation of the effects of this feature on the dose calculations in Nagra (2010a).

The first two aspects of VPAC 1.1 verification are described in detail in Holocher et al. (2008) and are summarised only briefly in the following.

Verification of the treatment of the main processes in VPAC 1.0

Key elements of VPAC were individually assessed with respect to their correctness and functionality by means of a comprehensive set of test cases, independent solutions of which had been derived either analytically or by using other computer codes. In particular, the following tests were made.

- The flow evaluation was tested using the case of unsteady well flow, for which an analytical solution exists.
- The implementation of the nuclide source term was tested by considering the release of I-129 from spent fuel to a canister interior, without considering transport into the surrounding buffer. The results for the three waste geometries implemented in VPAC were then compared with the corresponding analytical solutions.
- The treatment of decay and decay chains was tested by considering the release of radionuclides in a section of the 4n+2 decay chain from spent fuel to a canister interior, again without considering transport into the surrounding buffer. In this case, VPAC results were compared with those using the near-field code STMAN 5.7 (Robinson 2009).
- The treatment of solubility limitation was tested by extending the above example to include solubility limitation of Am and Th, and then comparing the radionuclide concentrations with those calculated using STMAN 5.7.
- The treatment of diffusion and sorption was tested by including the additional processes of buffer diffusion and sorption in the above example. Results for both constant and time-dependent sorption coefficients and also for both constant and time-dependent diffusion coefficients were compared with results calculated using STMAN 5.7. Note that STMAN can also handle time-dependent diffusion and sorption parameters (see Section 3.4.3).
- The treatment of advection and dispersion was tested using two test cases: (i) a semi-infinite homogeneous porous medium with a fixed concentration boundary condition at the upstream boundary for a single radionuclide, and (ii) a homogeneous porous medium of finite extent in the flow direction with a more complicated time-dependent source term for a radionuclide decay chain (a section of the 4n+2 decay chain). The results of test case (i) were compared with the corresponding analytical solution. The results of test case (ii) were assessed against the results calculated using PICNIC 2.4 (Robinson 2004).

In each test case, close agreement was found between the VPAC results and the corresponding analytical solution or the STMAN / PICNIC results. More details on the verification of the treatment of the main processes in VPAC 1.0 are given in Chapter 4 of Holocher et al. (2008).

Benchmark tests for VPAC 1.0

Two sets of benchmark tests were carried out: one where an analytical solution is available and another where VPAC results were compared with the results of the SEFTRAN code (Ward et al. 1988)[30]. The benchmark tests addressed more realistic cases than the rather abstract test cases used for the verification of the treatment of the main processes.

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[30] SEFTRAN, or *Simple, Efficient and Fast Transport Model*, is a 2D finite element code. It can handle single radionuclides, but not radionuclide chains (i.e. it does not account for ingrowth). Furthermore, it cannot deal with limited elemental solubility and is restricted to instantaneous radionuclide release from a waste form. SEFTRAN is a verified code that has been extensively used in the long-term safety assessments carried out in the course of a L/ILW repository project at the Wellenberg site (Nagra 1994).

The first set of benchmark tests concerns vertical upward groundwater flow passing through an emplacement cavern (Fig. 3-4). The nuclides are, in the first test, released from the cavern into the undisturbed host rock (hereafter named rock matrix, see cross section M – M' in Fig. 3-4). In the second test, nuclides are additionally released into two discrete vertical fractures (hereafter named disturbed zones, see cross section D-D' in Fig. 3-4).

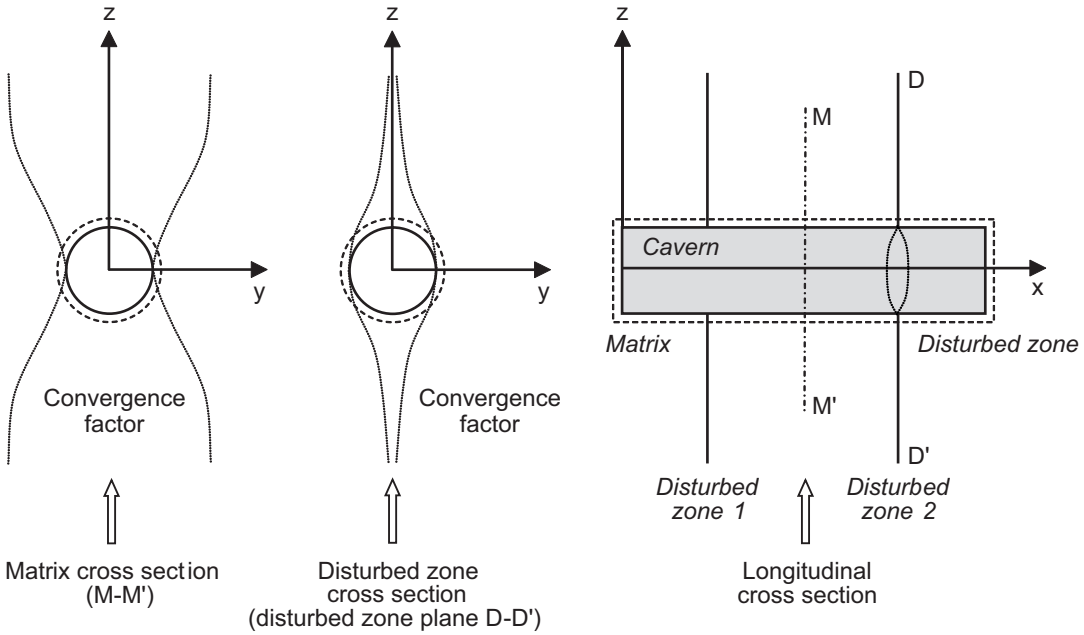

Fig. 3-4: Conceptual models for analytical benchmarks for VPAC 1.0 (adapted from Figure 5.2-1 in Holocher et al. 2008).

The maximum fractional release rates at 1 m distance from the emplacement cavern calculated with VPAC generally agreed well with analytical calculations for all rock matrix hydraulic conductivity values and fracture transmissivity values considered. The most pronounced difference was found in case of a highly permeable rock matrix with fractures. Here, a significant interaction between the undisturbed rock matrix and the fractures was identified in the VPAC calculations. This interaction is, however, omitted in the derivation of the analytical solutions, which simply assume independent, additive transport in the undisturbed rock matrix and in the fractures.

The second set of benchmark tests addressed a cylindrically symmetrical representation of a L/ILW cavern containing a series of waste containers (Fig. 3-5). At one end of the cavern, a branch tunnel and a transfer area were also modelled. In these test cases, groundwater flow occurs horizontally from the left side of the model area to the right side. Two test cases were considered: one in which the host rock is undisturbed and another one in which the cavern is intersected by two fault zones, arranged as shown in Fig. 3-5.

The results of VPAC and SEFTRAN for the defined test cases were found to be in close agreement. More details of the benchmark tests for VPAC 1.0 can be found in Chapter 5 of Holocher et al. (2008).

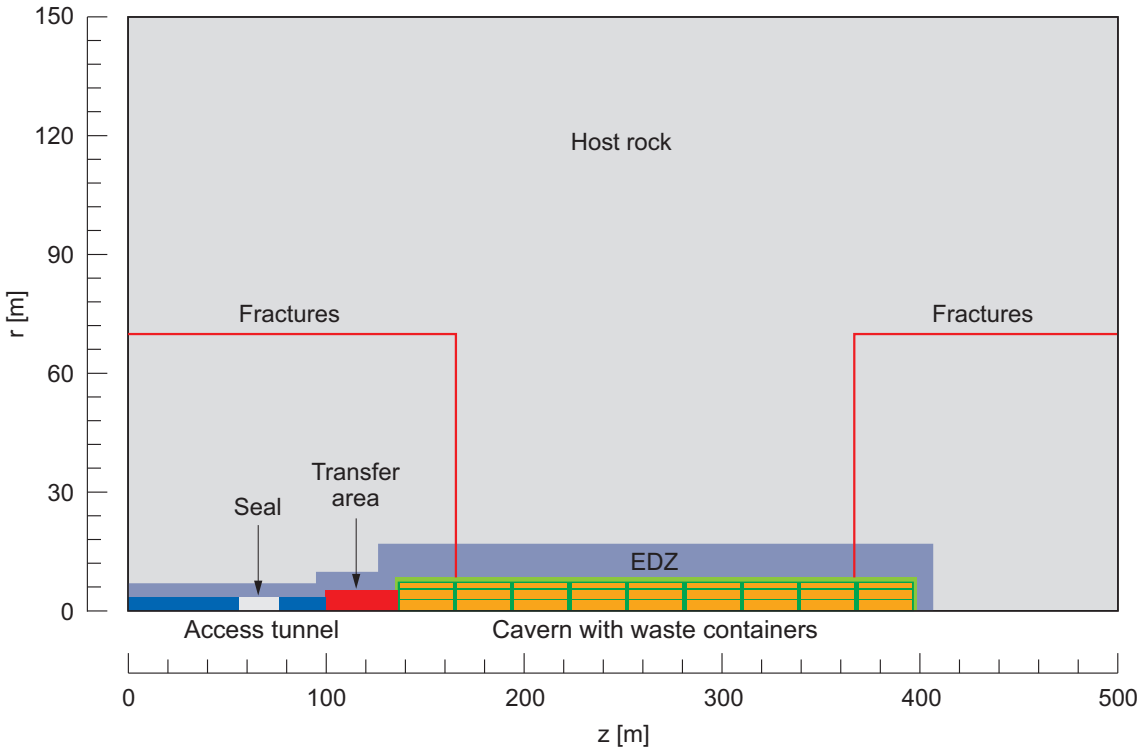

Fig. 3-5: Conceptual model for benchmark tests in which VPAC 1.0 and SEFTRAN results are compared (adapted from Figure 5.3-1 in Holocher et al. 2008).

Recalculation of selected calculation cases from an earlier safety assessment

After official release, VPAC 1.1 was successfully installed and the complete set of VPAC calculations as part of the dose calculations in Nagra (2010a), was recalculated in an automatic manner. The results are identical to those obtained with VPAC 1.0.

Test of the new anisotropic diffusion capability in VPAC 1.1

A simple 3D test case was designed to test the new anisotropic diffusion feature of VPAC 1.1. In this test case, a nuclide is assigned a specific initial concentration within a single model element at the origin of a 3D cubic model domain, into which it then diffuses. The diffusion tensor was chosen such that diffusion along one model axis is four times faster than along the other axes. The correct functioning of the new feature was confirmed by comparing the calculated concentration profiles along the various axes.

Following this, the effect of anisotropic diffusion in the host rock on near-field release and geosphere release was investigated in selected calculations for the L/ILW repository in Nagra (2010a). The results show that this process has a discernible effect on near-field release. However, the effect on radionuclide release from the geological barriers is small.

3.4 The STMAN suite of codes

3.4.1 Scope and purpose

STMAN is a family of three computer codes that model the release of nuclides from different waste forms and subsequent 1D radial transport through the engineered barriers. The three codes are:

- SPENT, which is applicable to directly disposed of spent fuel (SF),
- STRENG, which is applicable to vitrified high-level waste (HLW), and
- STALLION, which is applicable to long-lived intermediate-level waste (ILW) and to low- and intermediate-level waste (L/ILW).

STMAN has been enhanced iteratively following its initial development, based on experience gained through its application in several Nagra projects. Successive versions of STMAN have been documented in a series of User Guides, Release Notes and Technical Notes on the mathematical model provided by the developer. STMAN Version 5.9 has recently been released (Robinson 2013).

Radionuclide transport calculations are carried out easily and quickly using STMAN. The code provides accurate numerical solutions for simple geometrical problem settings. Note that, in many cases, simplified geometrical representations of more complex systems are adequate for the purposes of safety analysis, especially given the uncertainties in the values assigned to the input parameters. In some cases, however, simplifying complex geometrical settings such that they can be handled using STMAN may mean that the desired level of accuracy is not reached. The use of STMAN in the present dose calculations is explained in Section 5.3.6.

3.4.2 The model domain

A single canister (SPENT and STRENG) or a single emplacement cavern (STALLION) is usually modelled. Up to three sub-domains may be distinguished:

(i) the waste form or the water-filled space[31] to which nuclides are first released,

(ii) an optional surrounding annular region of buffer material[32], through which nuclides are transported by radial diffusion and which can be divided into an arbitrary number of concentric sub-regions, each having its own specific transport properties, and

(iii) an optional host rock layer, which is a 1D linear abstraction of the host rock surrounding the waste form and the buffer material.

All sub-domains (i) to (iii) are conceptualised as homogeneous porous media (see Sections 3.1 and 3.2).

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[31] This is the void space inside the disposal canisters – termed the reservoir – in the case of SF and HLW and the pore space of the porous waste forms in the case of ILW and L/ILW.

[32] For SF and HLW, the buffer material consists of bentonite. For ILW and L/ILW, there is no buffer material present and the thickness of this domain is set to zero.

3.4.3 Processes and parameters

Processes explicitly included in STMAN are:

- a period of complete containment, e.g. in a SF / HLW disposal canister,
- release of nuclides (radionuclides and stable isotopes) from the waste matrix, which can be time dependent,
- radioactive decay and ingrowth, with an unlimited number of radionuclides and unlimited decay chain lengths,
- 1D radial diffusion of nuclides from the waste form through the buffer material (if present) to the host rock (if present), with diffusion coefficients in the buffer material that can be time dependent,
- advective / dispersive / diffusive transport of nuclides in the 1D linear representation of the surrounding host rock,
- nuclide-specific linear sorption equilibrium between the liquid and solid phases, with sorption-coefficients that can be time-dependent, and
- element-specific solubility limitation, with solubility limits that can be time dependent.

The codes SPENT and STRENG are also able to model the situation in which a breached disposal canister provides some resistance to nuclide transport into the buffer material. This feature is implemented in the form of one or more pinhole-type breaching points. The possible ejection of water from the canister interior and through the buffer, e.g. due to a build-up of gas pressure, may also be modelled. However, neither feature is used in the dose calculations performed for SGT Stage 2. The reader is referred to Robinson (2008) for details of the pinhole option and the model of water ejection pulses.

There are two broad options available to the user regarding the interface between the buffer material and the host rock:

(i) to specify a boundary condition, of which two types are available, and

(ii) to use the optional host rock layer.

With regard to option (i), the simplest type of boundary condition is a fixed concentration condition, for which the value is usually set to zero. Alternatively, a mixing-cell boundary condition can be used. This type of boundary condition assumes that the diffusive nuclide flux across the interface between the buffer material and the host rock is balanced by an effective advective nuclide flux in the host rock. The concentration in the mixing-cell (i.e. at the interface between the buffer material and the host rock) is then set dynamically by the code to maintain the balance. The water entering the mixing-cell from upstream in the host rock may have a user-specified nuclide concentration or may carry a user-specified nuclide flux. In the latter case, the user-specified nuclide flux is read from a separate input file. The groundwater flow rate in the host rock may also be specified by means of a separate input file.

The option with the host rock layer (ii) is motivated by the need to obtain satisfactory estimates of nuclide releases across the interface between the buffer material and the host rock in cases where diffusive transport in the rock is significant, and nuclides are therefore transported not only from the buffer to the rock but also vice versa. The layer is thus sometimes also referred to as the *diffusive host rock layer*, although advective transport in the host rock may also be taken into account. Generally, the same transport processes as in the buffer material are modelled in the host rock layer, although solubility limitation is conservatively disregarded. Moreover, the host rock layer is represented by a 1D linear (Cartesian) geometry, whereas the buffer is represented by a 1D cylindrical geometry. The surface area between the buffer and the host rock

is set equal to the outer surface area of the buffer material. The host rock layer has a specified length and the boundary condition at the far end is one of zero concentration. The lower part of Fig. 5-4 shows how this option is used in the general modelling approach.

3.4.4 Solution method

The solver used in STMAN 5.9 is a Differential-Algebraic Equation Solver known as DYLAN. It uses a backward difference, variable order time-stepping scheme based on the method described by Byrne & Hindmarsh (1975). The discretised equations solved by DYLAN are a combination of differential and algebraic equations for the concentrations, fluxes and amounts of each nuclide. They are described in detail in Robinson (2013).

The sub-domains are each discretised into a number of cells with varying sizes. The numbers of cells used for the buffer material and the host rock layer are set by the user. Generally, increasing the number of cells improves the accuracy, although typically a few tens of cells for each sub-domain are sufficient.

3.4.5 Input requirements

Input parameters for each STMAN calculation are specified in a so-called problem file with flexible formatting but specific keywords. A detailed description of the problem file syntax is given in Robinson (2013).

Parameter values given to STMAN must have units explicitly stated. The units must be convertible to the internal units of the code. Note that only the physical and chemical parameters that are related to release from the waste form to the reservoir or to the cementitious region are specific to SPENT, STRENG or STALLION. The other parameters apply to all STMAN codes. Besides the physical and chemical input parameters for the different sub-domains, the problem file also includes a number of control variables, e.g. to control the accuracy of the solution, to provide the code with pre-defined output times or to select the desired option for buffer / host rock interface. Tab. 3-3 lists the most important input parameters.

The groundwater flow in the host rock layer may be constant or time dependent. In the former case, the flow rate is given in the problem file. In the latter case, flow rates are read from a separate file. There is, however, no facility for making diffusion in the host rock layer time dependent.

Steady or time-dependent solubility limits, sorption coefficients, diffusion coefficients and, in the case of SPENT, fractional release rates from the spent fuel matrix and the cladding are also specified in the problem file. In the case of STRENG, the glass dissolution model follows the approach to modelling a fragmented glass block as a number of equal spheres (see Section 3.2.3). In the case of STALLION, it is possible to specify a fraction of the inventory of each nuclide that undergoes gradual release (e.g. congruent release due to the slow corrosion of certain metallic waste forms at a constant rate). The remainder of the inventory is released instantaneously.

STMAN has a restart capability, whereby separate runs may be carried out for successive periods of time, allowing physical and chemical parameters values to be altered between consecutive runs.

Tab. 3-3: STMAN input parameters.

Parameters required only by individual codes are indicated using with abbreviated code names: SP (SPENT), SG (STRENG), SN (STALLION). ALL denotes applicability to all three codes.

Parameter	**Symbol**	**Dimen-sion**	**Code**	**Element- (E) or nuclide-specific (N)**	**Time-dependent**
Nuclide and inventory data					
Radionuclide half-life	$T_{1/2} = \frac{\ln 2}{\lambda^N}$	T	ALL	N	
Branching ratio	σ^{BN}	-	ALL	N	
Instant release fraction (SP) or fraction of ILW inventory undergoing instant release (SN)	IRF^N	-	SP, SN	N	
Fraction of initial inventory associated with the fuel and the cladding	N_m^N/I^N	-	SP	N	
Total initial inventory	I^N	M	ALL	N	
General physical and chemical parameters					
Containment time	t_c	T	ALL		
Length of modelled unit (single disposal canister or single cavern)	L_C, L	L	ALL		
Number of modelled units (canisters or caverns)	-	-	ALL		
Initial diameter of waste form (used to calculate reservoir volume, see below)	r_0	L	SP, SG		
Total porosity for cement (SN) and the host rock layer	ε	-	ALL		
Glass matrix density	ρ	M/L^3	SG		
Glass dissolution rate	r	M/(L^{2}T)	SG		
Equivalent radius of glass spheres	r_s	L	SG		
Fractional release rate due to dissolution / corrosion of spent fuel and cladding (SP) or fractional release rate for the slow release fraction in SN	$f_m(t)$	1/T	SP, SN		✓
Grain density or bulk dry density for cement (SN only), buffer material and host rock	$\frac{\rho_s}{1-\varepsilon}$ or ρ_s	M/L^3	ALL		
Reservoir thickness	$r_0 - \sqrt{r_0^2 - \frac{V_R}{\pi \cdot L}}$	L	SP, SG		

Tab. 3-3: (continued)

Parameter	Symbol	Dimen-sion	Code	Element- (E) or nuclide-specific (N)	Time-dependent
Water flow, solute transport and retention parameters					
Solubility limits for the reservoir or the cavern	c_{sol}^{E}	M/L^3	ALL	E	✓
Sorption coefficients for the cavern (SN only) and the host rock	K_d^E	L^3/M	ALL	E	✓
Nuclide concentration in incoming groundwater for fixed concentration and mixing-cell boundary conditions	c_{GW}^{N}	M/L^3	ALL	N	
Nuclide flux in incoming groundwater for mixing-cell boundary condition	f_{GW}^{N}	M/T	ALL	N	✓
Groundwater flow rate	Q	L^3/T	ALL		✓
Host rock (effective) diffusion coefficient	$\varepsilon^E D_p^E$	L^2/T	ALL	E	
Host rock porosity factor	$n^E\ (=\frac{\varepsilon^E}{\varepsilon})$	-	ALL	E	
Physical and chemical parameters that can be specified separately for each buffer region					
Buffer (effective) diffusion coefficient	$\varepsilon^E D_{p,BM}^E$	L^2/T	ALL	E	✓
Buffer total porosity	ε	-	ALL		
Buffer grain density or bulk dry density	$\frac{\rho_s}{1-\varepsilon} or\ \rho_s$	M/L^3	ALL		
Buffer solubility limits	c_{sol}^{E}	M/L^3	ALL	E	✓
Buffer sorption coefficients	K_d^E	L^3/M	ALL	E	✓
Buffer porosity factor	$n^E\ (=\frac{\varepsilon^E}{\varepsilon})$	-	ALL	E	

3.4.6 Verification

General

Verification of the STMAN suite of codes was performed in two stages. Firstly, full scale comparisons of STMAN results with the results of other codes or with analytic solutions were carried out. Secondly, the behaviour of new capabilities was tested as the code was developed from one version to the next. A simple test for the capability to have several buffer sub-regions is described in the STALLION verification section below, but is applicable to STMAN as a whole. Testing of the current version 5.9 of STMAN is described in the Release Notes for Version 5.9.

The STMAN codes were completely re-written in 1999, the earlier versions being written in FORTRAN and the later (and current) versions being written in C++. Because there was no common code between the versions, the successful cross-comparison between them provided strong confirmation of their correct functioning. The new versions had more accurate discretisation than the older ones, so the results were not identical; a range of discretisations was tested to confirm that this was the only cause of any differences.

The individual STMAN codes differ only in their treatment of the waste forms and the associated processes. The major part of the codes, involving transport through the buffer and interfacing to the host rock, is common. Verification of any of the codes is, in this regard, verification of all of them. In the case of a strongly solubility limited nuclide, which maintains a constant concentration in the waste form, all of the codes are expected to produce the same release profiles, since the waste form aspects are irrelevant.

Recent verification steps have been the recalculation of selected calculation cases from the latest officially approved safety assessment in Nagra (2010a) and detailed tests of the new capability to evaluate the near-field release within the host rock layer.

Verification of SPENT

The original version of SPENT was verified by cross-comparison with the PAGODA code. PAGODA is an integrated performance assessment tool which has been used for strategic and training purposes, but is capable of producing a good approximation to the spent-fuel release and buffer transport aspects in SPENT. Good agreement was obtained for a complete decay chain (Brown & Williams 1993).

A detailed cross comparison was undertaken between SPENT and AMBER in the context of a larger cross-comparison exercise in 2001 (Little et al. 2003). This took an extended list of radionuclides and two types of spent fuel (with different properties). AMBER is a general-purpose compartment modelling tool that can be used to create compartment models for transport of radioactive contaminants (Quintessa 2010). A specific compartment model was constructed to reproduce the SPENT model, so that good agreement would be expected. A mixing-cell boundary condition was applied in the SPENT model.

Fig. 3-6 shows the STMAN and AMBER results for the release of key radionuclides from the buffer into the host rock for one of the waste types. They match very well, and other results were in similarly good agreement.

The comparison exercise actually went further than the verification of SPENT, because the AMBER model included a far-field component. It was therefore possible to verify SPENT and PICNIC linked together against an integrated compartment model of the full system. Geosphere release rates were converted to dose rates using the same biosphere dose conversion factors. Figs. 3-7 and 3-8 show the results produced by SPENT/PICNIC and by AMBER, respectively. They are in good agreement.

Verification of STRENG

Verification cases for the original version of STRENG were documented by Grindrod et al. (1990). These involved comparison with analytical solutions for transport problems with single solubility-limited radionuclides and internal cross-checks for transport problems with decay chains. The key difference between STRENG and SPENT is in the waste dissolution models. These models are sufficiently simple that hand checks on the reported amounts of nuclides in the various locations distinguished by the model (glass and reservoir) were able to confirm the correct functioning.

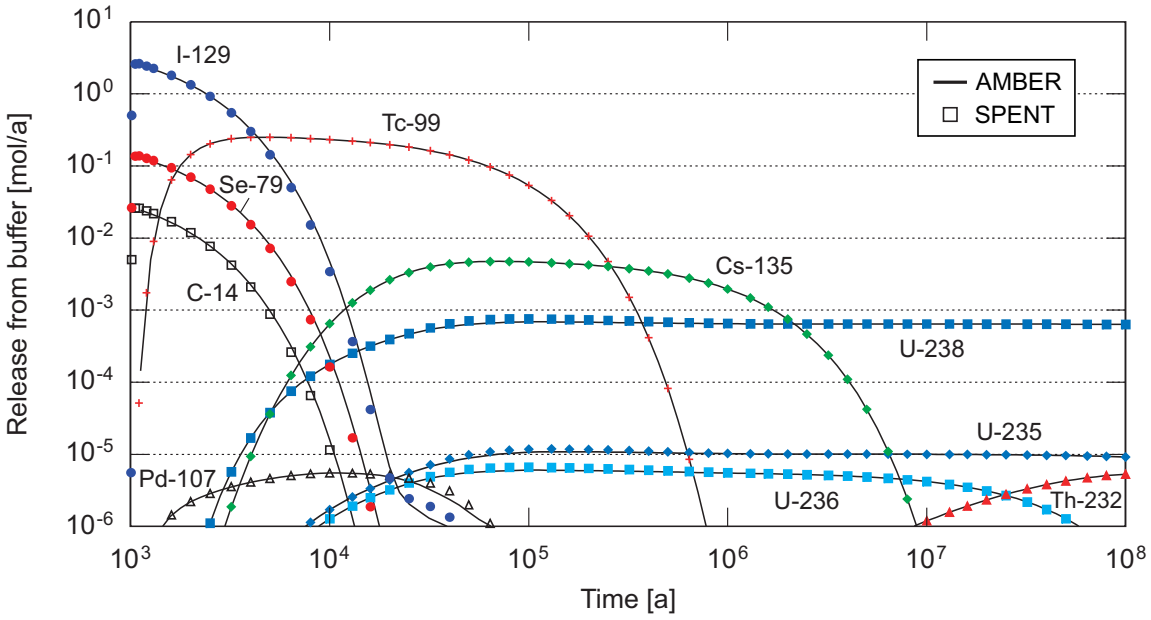

Fig. 3-6: Comparison of SPENT and AMBER results in a code comparison exercise.

Verification of STALLION

Verification cases for the original version of STALLION involved comparison with analytical solutions for transport problems with single solubility-limited radionuclides and internal cross-checks for transport problems with decay chains.

The key difference between STALLION and the other STMAN codes is in the waste model. The inner sub-domain of the STALLION model is a uniformly mixed domain. Thus, simple hand checks can be carried out on the concentrations and on the sorbed and precipitated amounts. Some radionuclides can have a slow-release fraction. A specific test case for two example radionuclides, C-14 and Cl-36, was set up to test this feature, in conjunction with a thin buffer giving rapid release to the geosphere. The test is documented in the Release Note for STMAN Version 5.4.5. With a slow fractional release rate of 10^{-4} a^{-1}, the remaining unreleased inventory at 1'000, 10'000 and 50'000 years was compared with the analytical result and very good agreement was obtained.

As noted above, verification of new capabilities of the STMAN suite of codes was undertaken with each new release. This generally involves hand calculations to confirm successful operation. In the case of the capability to model several buffer sub-regions, which was first implemented in STMAN 5.7, a comparison test with two buffer layers was run against the AMBER compartment modelling tool. This used a single radionuclide that was solubility limited throughout. The outer part of the buffer had a higher porosity and a higher effective diffusion coefficient.

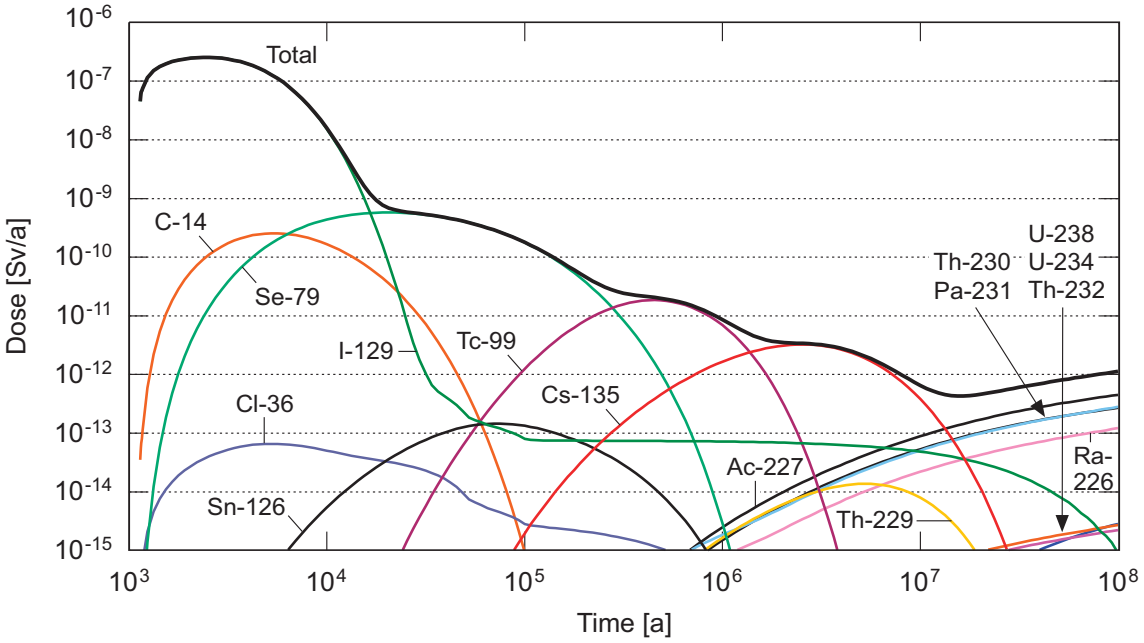

Fig. 3-7: Dose rates calculated using SPENT and PICNIC in a code comparison exercise.

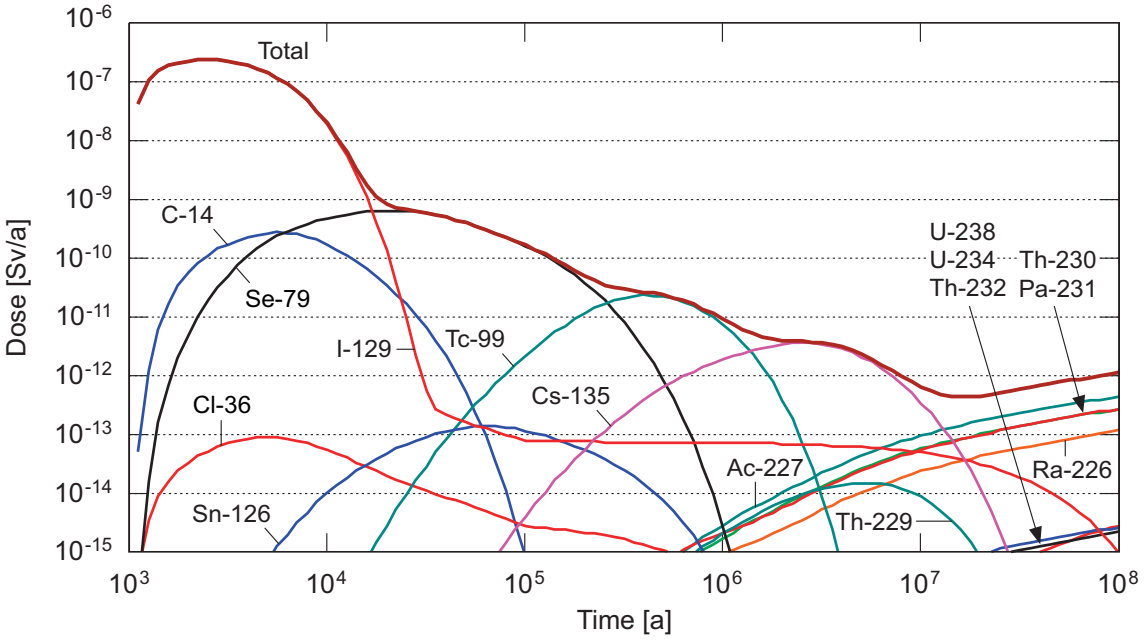

Fig. 3-8: Dose rates calculated using AMBER in a code comparison exercise.

Fig. 3-9 shows a direct comparison for the case in which the AMBER compartment model was tuned to match the numerical discretisation used in STALLION. The resulting agreement is excellent (4 significant figures except at very early times when the release is tiny). Testing of the capability of STMAN to model more than two buffer sub-regions is reported in the Release Note for Version 5.8.

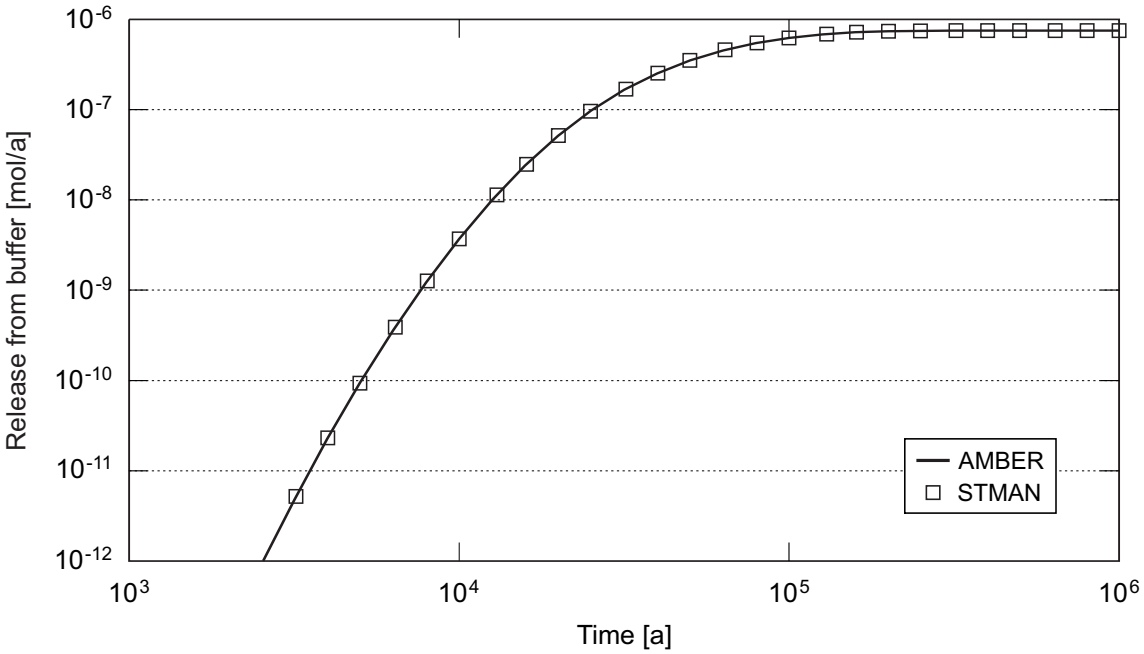

Fig. 3-9: Comparison of STMAN (STALLION) and AMBER buffer release rates in a code comparison exercise.

Recalculation of selected calculation cases from an earlier safety assessment

After its official release, the earlier version STMAN 5.8 was successfully installed and the complete set of STMAN calculations as part of the dose calculations in Nagra (2010a), was recalculated in an automatic manner. The results were identical to those obtained with STMAN 5.7.2, which is the version used for the original calculations in Nagra (2010a). Later, selected cases of Nagra (2010a) were repeated with the latest version 5.9 and correct operation was confirmed.

Testing of new capabilities

The new capability of evaluating the near-field release within the host rock layer was first introduced in code version 5.8. The effect of this feature on near-field release was then investigated using selected calculations for the HLW repository in Nagra (2010a). The results showed that near-field release is slightly lower when evaluated within the host rock layer. However, the effect on radionuclide release from the geological barriers is negligible.

The current version STMAN 5.9 has the additional capability of calculating the spatially integrated nuclide masses on either side of the position in the host rock layer where near-field release is reported. Testing confirmed that the new feature functions correctly.

3.5 The PICNIC / PICNIC-TD codes

3.5.1 Scope and purpose

PICNIC is a computer code that models transport of dissolved nuclides along a porous, water-saturated 1D linear transport path. Multiple paths may be connected to form a network model. These transport paths are called legs in PICNIC. Each leg can be parameterised such that it represents either a homogeneous porous medium or a discrete water-conducting feature, including the adjacent porous rock matrix, using the modelling approach described in Section 3.2.7. With this flexibility, PICNIC is capable of modelling the rather heterogeneous flow and transport systems that may be present in the geosphere as a network of legs.

The original version of PICNIC (Barten & Robinson 2001) used a fast numeric solver based on the Laplace transform method and did not require any spatial discretisation along the legs. However, the latest version of PICNIC, termed PICNIC-TD, which has the additional capability of handling time-varying groundwater flow and nuclide transport in the matrix parallel to a water-conducting feature, does require spatial discretisation.

Successive versions of PICNIC have been documented in a series of User Guides, Test Reports and Release Notes provided by the developer. The mathematical model for the most recent version of PICNIC-TD (Version 1.4) is described in an appendix to the User Guide (Robinson & Watson 2013) and in the following sections.

PICNIC-TD (and PICNIC) are well-suited to problems in which radionuclide transport can be considered to occur predominantly along a one-dimensional linear flow path. In most cases, the assumption of one-dimensional linear flow paths is a significant simplification of reality, e.g. due to the non-uniform distribution of radioactive waste in the repository. However, for post-closure safety analysis, which is often based on simplifications and pessimistic assumptions (especially at early stages of repository planning), the assumption of one-dimensional and linear transport is considered adequate if, at the same time, spatially averaged properties of the model domain are used (see also Section 5.4.5).

3.5.2 The model domain

PICNIC-TD legs are used primarily to represent one-dimensional transport paths through a heterogeneous geosphere, but may also be used to model different underground structures of a deep geological repository like branch tunnels, ramps, shafts and seals.

Every leg has an upstream end and a downstream end, referred to as a junction, where it may, or may not, be connected to further legs or other model features. In particular, a junction may have one or more incoming or outgoing legs. However, some have no incoming legs, but are connected to a source term (typically an STMAN or VPAC output), while others have no outgoing legs, but produce a result. Legs may optionally produce additional diagnostic outputs (e.g. total mass) for positions within a leg. Fig. 3-10 illustrates an example network, with the different types of junction mentioned.

Each PICNIC-TD leg models a pair of spatially distinct elements: a discrete flow feature and the adjacent lower permeable rock, called matrix (double-porosity model, see Section 3.2.7). The flow features themselves may contain infill material, which allows PICNIC-TD legs to be used to model homogeneous porous media. In this case, the matrix is omitted.

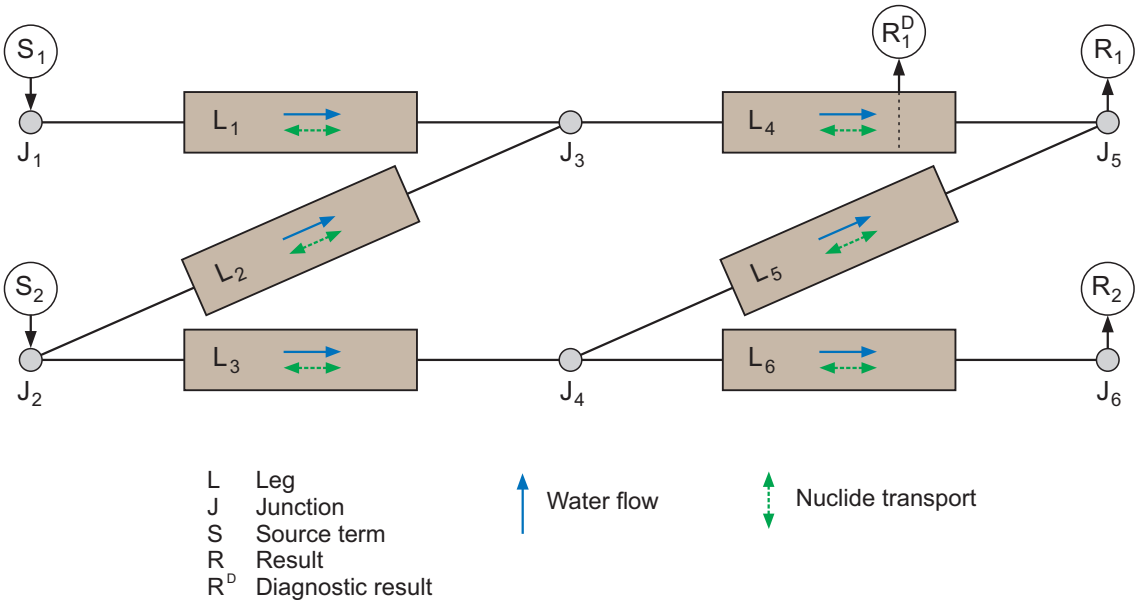

Fig. 3-10: An example of a PICNIC-TD network.

Two types of geometry can be handled: planar flow features (e.g. fractures) and cylindrical flow features (e.g. tubular structures, such as veins or tunnels). The matrix occupies a limited accessible region around these flow features (e.g., in the case of planar features, the matrix on either side is considered to have a thickness $(B - b)$; see Fig. 3-3).

The matrices of consecutive legs can be either linked or unlinked. If the matrices are unlinked, then all transported nuclides emerging from the matrix and the flow feature at the downstream end of the first leg are routed through the connecting junction, conceptualised as a point, where they are mixed. If the matrices are linked, then nuclides are transferred directly from the matrix of the upstream leg to the matrix of the downstream leg, with transfer between flow features handled in a similar manner.

3.5.3 Processes and parameters

Processes explicitly included in PICNIC-TD 1.4 are:

- radioactive decay and ingrowth, with an unlimited number of radionuclides and unlimited decay chain lengths,
- one-dimensional advective / dispersive / diffusive solute transport through the flow feature of a leg.
- diffusive transfer of nuclides between the flow feature and the adjacent matrix,
- diffusive transport of nuclides in the matrix perpendicular to the direction of flow and advective / dispersive / diffusive transport of nuclides parallel to the direction of flow, and
- nuclide-specific equilibrium sorption between liquid and solid phases.

From version 1.3 on, PICNIC-TD has been capable of handling non-linear as well as linear sorption equilibrium between liquid and solid phases for single nuclides or groups of nuclides. Only linear equilibrium sorption is, however, modelled in the dose calculations for the provisional safety analyses.

3.5.4 Solution method

In PICNIC-TD, the governing equations for radionuclide transport are spatially discretised for numerical solution at each time step. The algorithm for time-stepping is a variable order predictor-corrector method (Byrne & Hindmarsh 1975). This approach has been used successfully in, among many other codes, the STMAN suite (see Section 3.4.4), although PICNIC-TD uses a newer implementation than that used in STMAN.

3.5.5 Input requirements

Input parameters for each PICNIC-TD run are contained within a so-called problem file. A detailed description of the problem file syntax is given in Robinson & Watson (2013). Parameters defined in the problem file include a number of control variables (e.g. to control the accuracy of the solution and to specify desired output times), as well as the physical and chemical parameters summarised in Tab. 3-4.

Parameter values given to PICNIC-TD must have units explicitly stated. The units must be convertible to the code internal units. The units are specified in the same way as for STMAN and SwiBAC. A full description is given in the current User Guide (Robinson & Watson 2013).

Each leg is associated with a rock type, which defines a number of its properties. Several legs may share the same rock type. Every rock type includes a flow feature and its matrix, each with its own block of parameters. In addition, a number of further parameters not linked to the rock type or to the flow and matrix blocks are required to fully define the properties of a leg. These include its length and the flow rate, or Darcy velocity, of the water that passes through it. The Darcy velocity or flow rate through a leg may by specified in the problem file, or in a file containing information for determining a time-dependent Darcy velocity or flow rate. Other physical and chemical parameters are restricted to being time-independent. Retardation and retention parameters are specific to the flow and matrix blocks of individual legs and can either be set directly (via a base retardation or retention factor) or calculated from basic physical parameters, including porosity and sorption coefficients.

Tab. 3-4: PICNIC-TD input parameters.

Parameter	Symbol	Dimension	Element- (E) or nuclide-specific (N)	Time-dependent
Nuclide parameters				
Radionuclide half-life	$\ln 2 / \lambda^N$	T	N	
Branching ratio	σ^{BN}	-	N	
Leg parameters				
Length	l	L		
Cross-sectional area (CSA)	A	L^2		
Darcy velocity (flow block and matrix block)	q_L, q	L/T		✓
Peclet number (flow block and matrix block)	Pe	-		

Tab. 3-4: (continued)

Parameter	Symbol	Dimension	Element- (E) or nuclide-specific (N)	Time-dependent
Pore diffusion coefficient for flow block	D_L	L^2/T		
Effective diffusion coefficient for flow block (optional; otherwise calculated from component parameters)	$\varepsilon_L^E . D_L$	L^2/T	E	
Rock type parameters				
Flow / infill porosity	ε_L	-		
Specific surface area	δ_L	L^{-1}		
Penetration depth (for matrix diffusion)	$B - b$	L		
Flow block parameters				
Base retardation factor (optional; otherwise calculated from flow block infill porosity, density and sorption coefficients)	R_L^E	-	E	
Matrix block parameters				
Base retention factor (optional; otherwise calculated from matrix porosity, density and sorption coefficients)	R^E	-	E	
Matrix porosity	ε	-		
Porosity factor	$n^E \ (= \frac{\varepsilon^E}{\varepsilon})$		E	
Matrix pore diffusion coefficient perpendicular to flow	D_z^E	L^2/T	E	
Effective matrix diffusion coefficient (optional; otherwise calculated from component parameters)	$\varepsilon^E . D_z^E$	L^2/T	E	
Matrix anisotropy factor for diffusion	D_x^E / D_z^E	-	E	

In PICNIC-TD, a leg may represent a transport path that has several discrete and isolated flow features (including the adjacent matrix, see Fig. 3-11, left sketch). These discrete flow features may be either open channels or porous media (infill porosity). The input parameters cross-sectional area (CSA), Darcy velocity and flow porosity then refer to this combined transport path, including the rock between the individual flow features. In the dose calculations for the provisional safety analyses, the input parameters of such a leg are set in a different but equivalent way: the parameter cross-sectional area refers to the total cross-section of all discrete flow features (excluding the adjacent matrix, see Fig. 3-11, right sketch) and the flow porosity of the leg is equal to the infill porosity. Accordingly, the Darcy velocity is equal to that within the aggregated flow feature.

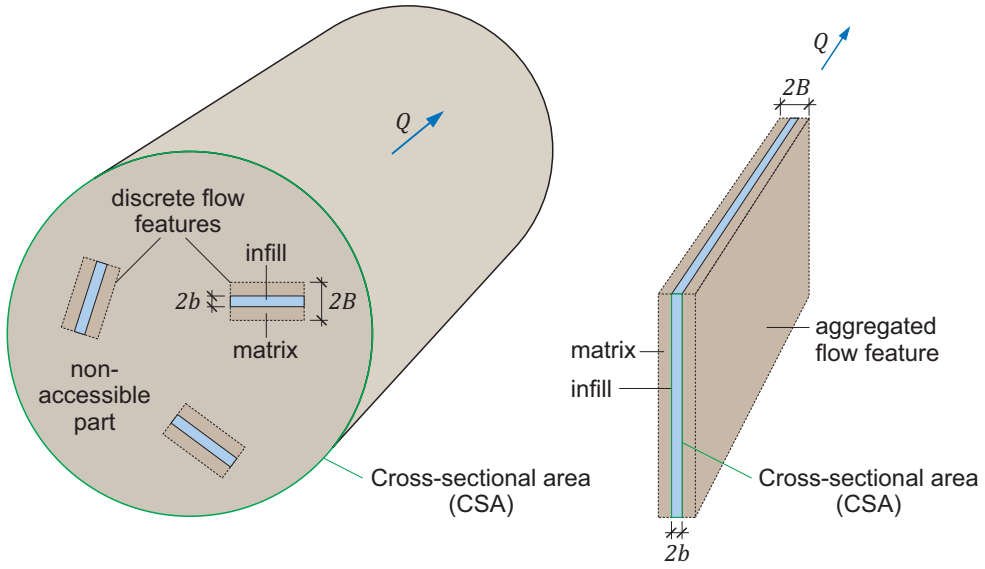

Fig. 3-11: Principal possibilities for the conceptual treatment of transport paths in PICNIC-TD for discrete planar flow features.
(left) Consideration of distributed but isolated flow features (including the adjacent matrix); (right) Aggregation of isolated flow features (approach used in the present dose calculations).

3.5.6 Verification

Verification of PICNIC / PICNIC-TD

The original implementation of PICNIC was extensively verified in a series of seven steps, with progressively greater complexity of the rock matrix (Barten & Robinson 2001). Later, PICNIC was also successfully tested in a cross-comparison exercise with AMBER (see Section 3.4.6).

PICNIC-TD was originally tested with selected cases from the comprehensive set of tests in Barten & Robinson (2001) and the test results are documented in the Release Notes of the successive versions. The latest version of PICNIC-TD (Version 1.4) has been shown to reproduce all test cases.

PICNIC-TD Version 1.3 was also tested against GEOTRAN-2D. This is a computer code that generates a semi-analytical solution for steady-state transport through a fractured porous medium, with one-dimensional water flow and solute transport in both the fracture and the matrix, and diffusive exchange between the two (see Section 3.2.7). Both codes were used to calculate fluxes of a set of example radionuclides into and out of the fracture and into and out of the matrix. Results are shown in Fig. 3-12. In general, good agreement is obtained between the results of the two codes. There are some differences observed for the sorbing nuclide Sn-126 when the standard spatial discretisation of PICNIC-TD is used. However, these differences virtually disappear when the spatial discretisation is refined.

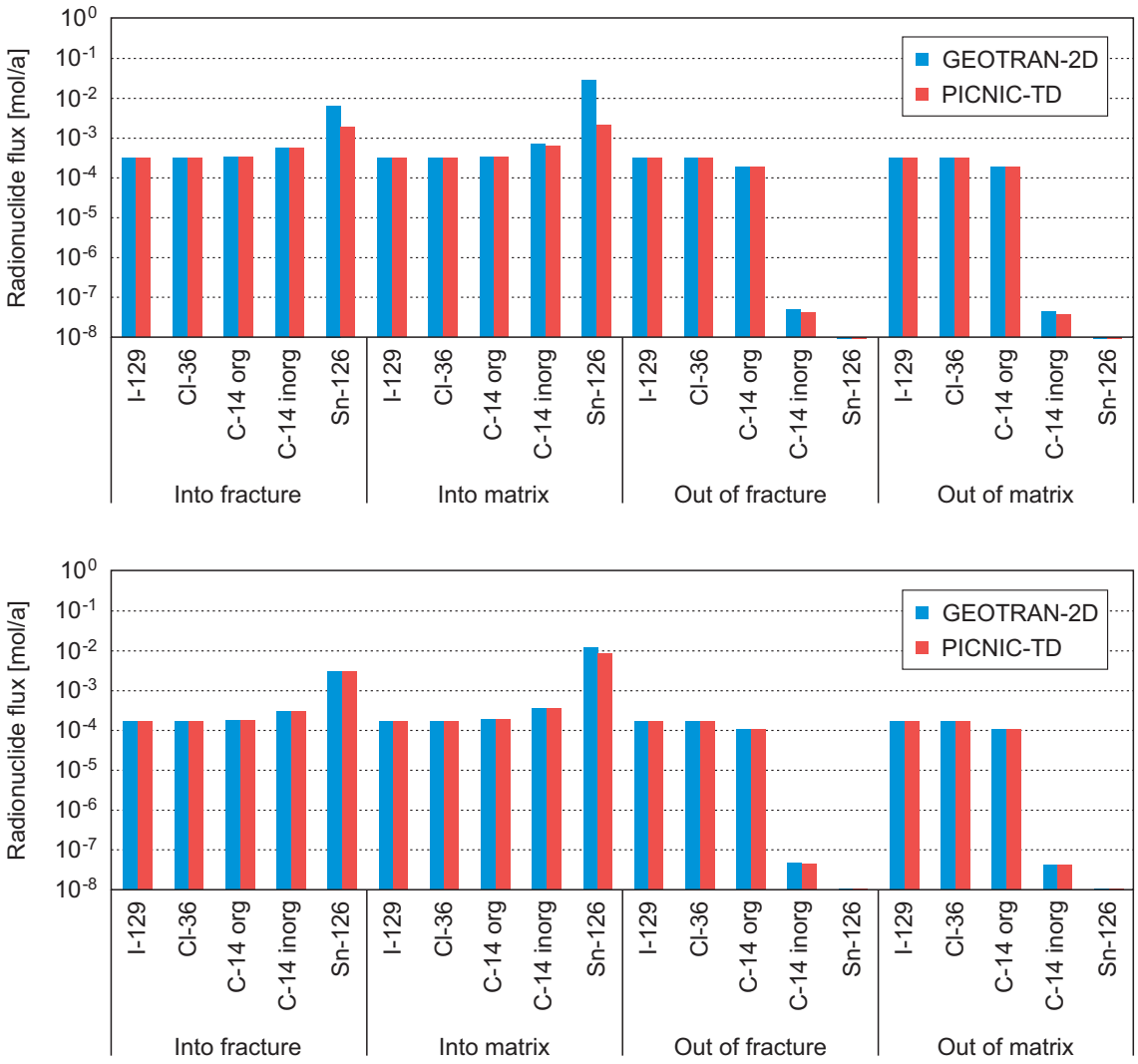

Fig. 3-12: Comparison of the results of PICNIC-TD and GEOTRAN-2D for steady-state transport through a fractured porous medium.
Standard spatial discretisation in PICNIC-TD (above); refined discretisation (below).

Recalculation of selected calculation cases from an earlier safety assessment

After its official release, the earlier version PICNIC-TD 1.3.3 was successfully installed and the complete set of PICNIC calculations as part of the dose evaluations in Nagra (2010a) was recalculated in an automatic manner.

The results were generally in good agreement. However, noticeable differences were observed for diffusion-dominated transport regimes. In these cases, the differences in the solution method (see above), i.e. the full coupling of consecutive legs in PICNIC-TD via shared nuclide concentrations at junctions versus the separate solution of transport for each leg in PICNIC, resulted in slightly higher or slightly lower nuclide fluxes from the final leg, depending on the ratio of the nuclide dependent effective diffusion coefficients in each of the linked legs. Overall, the results obtained with PICNIC-TD are considered to be more realistic than those calculated with PICNIC.

Later, selected cases of Nagra (2010a) were re-calculated with the latest version 1.4 and correct operation was confirmed.

Testing of new capabilities

New features added to the code, in particular the capability to handle flow and transport in the matrix parallel to flow direction in the discrete flow feature and the ability to handle non-linear sorption, were originally tested by the code developer. These tests are described in the Release Note for Version 1.3.

The effects of using these new capabilities have been investigated for selected calculations from Nagra (2010a). The results show that:

- linking the matrices of consecutive legs works as expected, and
- modelling a large-scale water conducting feature in a lower permeable homogeneous porous medium, with transport in the matrix parallel to flow direction, as well as diffusive exchange between the flowing feature and the matrix, results in a significant reduction of nuclide release from the geosphere when compared with the case where the flowing feature and matrix are modelled using two separate legs without diffusive exchange.

Prior to the development of PICNIC-TD, the latter approach (modelling the flowing feature and matrix with two separate legs without diffusive exchange) was the only way in which transport in the matrix parallel to flow direction could be included in PICNIC calculations.

The latest version PICNIC-TD 1.4 has a new feature for reporting of the time-history of mass leaving the model at any junction where nuclide concentration is specified (fixed concentration or file-based concentration). The mass can be defined simply as the time-integrated flux of a nuclide passing through the junction and out of the model. Alternatively, it can be defined as the amount of this nuclide that would exist outside the model at any time due to releases from the junction, taking radioactive decay and ingrowth outside the model domain into account. Testing confirmed that the new feature functions correctly.

4 Biosphere Modelling

This chapter provides an overview of the conceptual models and computer codes for calculating radionuclide migration and radiation exposure in the biosphere and highlights their interrelations with the relevant processes and parameters in Appendix A. It starts with a discussion of the regulatory requirements, a description of the underlying generic biosphere modelling concepts and a general model description in Section 4.1. Section 4.2 provides some key mathematical formulations of the general model. The implementation of the general model in the SwiBAC code is described in Section 4.3, along with references to more detailed documentation. The Nagra C-14 model (NC14M) is not described in detail; rather its most important aspects are described together with the SwiBAC code. The reader is referred to Nagra (2013) for a more comprehensive description of NC14M.

4.1 Modelling concepts and general model description

4.1.1 Regulatory requirements

The overall objective of deep geological disposal of radioactive waste is to ensure the long-term protection of humans and the environment from the effects of ionising radiation (ENSI 2009a). Generally, however, the environment is assumed to be sufficiently protected if the required measures for the protection of humans are taken (ENSI 2009b).

ENSI (2009a) provides both qualitative guiding principles and quantitative protection criteria for deep geological disposal that are consistent with this overall protection objective. The formulation of the protection criteria in ENSI (2009a) is founded on a number of international requirements and conventions, notably on IAEA (2006a,b), as well as on recommendations from the International Commission on Radiological Protection (ICRP 1998a, 2006, 2007) [33]. In the context of the provisional safety analyses in SGT Stage 2, protection criterion 1, which sets an annual individual limit to (effective) individual dose of 0.1 mSv, has to be met for the repository systems under consideration.

ENSI (2009a) further specifies that the annual individual dose referred to in protection criterion 1 relates to the radiation exposure of an average individual within the population group most affected by the potential impacts of the repository. This definition is equivalent to that given in the recommendations of ICRP (2006), which state that, for the purpose of a prospective dose assessment for a planned exposure situation [34], the dose to a representative person of the more highly exposed individuals of the population has to be calculated. According to ICRP (2007), the representative person should be considered to have habits and characteristics typical of this more highly affected group; the use of extreme assumptions based on a single individual should however be avoided.

ICRP (2006) gives a number of further recommendations on how the assessment of dose to the representative person should be carried out. For example,

- the more highly exposed group should be identified taking into account the expected spatial distribution of the radionuclides released from the source,
- all relevant exposure pathways should be addressed, and

[33] ICRP (2013), which is an update of ICRP (1998a) that refers to the latest recommendations in ICRP (2006, 2007), was produced after the publication of ENSI (2009a).

[34] In ICRP (2006), geological disposal is considered a planned exposure situation due to the deliberate production of the radioactive waste.

- the assessment should rely on assumptions that are plausible (i.e. consistent with everyday life experience), sustainable (e.g. with respect to diet and use of local resources) and homogeneous (e.g. with respect to the habits of the group under consideration).

The first of these recommendations leads to the standard approach for identifying the more highly affected group, whereby regions and time periods in which radionuclide concentrations in the environment are expected to be highest are considered. This approach has recently been confirmed by the latest recommendations in ICRP (2013).

According to ICRP (2007), prospective dose assessments for members of the public should normally be carried out for different age categories. For the specific case of geological disposal, however, it is argued that, due to the expected slow changes of environmental radionuclide concentrations, the calculation of an average lifetime dose is a reasonable measure of the radiological effects on humans in the distant future. Furthermore, this measure is adequately represented by the annual effective dose to an adult person.

ICRP (2013) distinguishes between different periods within the life cycle of a deep geological repository, based on the level of control over the radioactive material. For later periods with only indirect oversight or no oversight of this material, radiation exposures are treated as potential exposures. This term is also used in the present report.

Regulatory requirements that are specific to biosphere modelling in SGT Stage 2 are discussed in a specific reference report to Nagra (2014b).

4.1.2 Overall approach

In the context of the provisional safety analyses for SGT Stage 2, the biosphere is taken to include a limited area of the terrestrial surface inhabited by individuals of the population that are more highly exposed as a result of radionuclide release from the barrier system. Such areas are typically located in regions where discharge of deep groundwater from the geological siting regions may occur, since this is where radionuclide concentrations in the environment are expected to be highest. The biosphere model system for any such area includes the vegetation, livestock and other fauna present, the atmosphere and surface waters and, below ground, the soils and an underlying near-surface aquifer.

The key role of biosphere modelling in a typical post-closure safety assessment is to interpret radionuclide releases from the engineered and geological barrier system in terms of effective dose rates that can be used to test compliance with regulatory protection criteria. As outlined in the previous section, dose rates are calculated for a typical adult member of the population group that would receive the highest (additional) dose rates as a result of the presence of the repository. Since this group inhabits the area in which the highest concentrations of radionuclides released from the repository are expected to occur, site-specific biosphere models are developed for areas with possibly high radionuclide concentrations in the context of the provisional safety analyses for SGT Stage 2. These site-specific biosphere models are based on today's geomorphological, hydrogeological and climatic conditions and thus illustrate the effects of their present variability and serve to evaluate its safety relevance. On the other hand, significant geomorphological and climatic changes will almost certainly occur in the potentially affected areas over the assessment time frames. Due to the substantial uncertainties in these changes and their impacts, which are much greater than the present-day and expected future variability between the potentially affected areas, a generic biosphere system that is applicable to all geological siting regions is also considered. A generic biosphere system has the additional advantage that any differences in the post-closure performance of the engineered and geological barriers in the different siting regions are not masked by differences and uncertainties related to the biosphere and its evolution.

The regulations also state that the population group for which radiological exposures are calculated should have habits that are realistic based on a present-day perspective. Thus, a present-day average diet and present-day agricultural practices[35] are assumed. However, a number of additional assumptions are made to ensure that dose rates to the representative person are not underestimated. In particular, all food and drinking water is assumed to be produced locally in the area under consideration. This assumption limits any significant dilution with uncontaminated, external material and also avoids losses from the system, other than those considered in the biosphere model. Also conservatively, the members of the more highly affected group are assumed to spend their entire life times within the biosphere area under consideration. Together, these assumptions yield higher than realistically expected dose rates.

4.1.3 Surface conditions and their evolution

The potentially affected areas are not expected to be subject to marine influence throughout the time frames for safety assessment. Thus, a terrestrial, fresh-water ecosystem type used for agricultural production is selected for biosphere modelling. Steady-state climatic and geomorphological conditions (temperature, precipitation rates, river systems etc.) are assumed in any individual biosphere calculation. This is a stylised assumption since, as noted in the previous section, significant climatic and geomorphological change will almost certainly occur over the assessment time frames.

Present-day temperate climatic conditions are assumed in reference calculations for SGT Stage 2. In addition, the regulator requires the safety relevance of plausible alternative climate states to be examined in the provisional safety analyses (ENSI 2010b); at a minimum, a climate that is warmer and dryer than at present and a colder (ice-age) climate should be considered. In this report, the conceptual models and codes for the present-day climate and a warmer and dryer climate are described. The case of a colder climate with periglacial conditions is analysed using the same stylised approach as in Nagra (2002b) and is not described further in the present report. Glacial conditions are not considered, since neither subsistence farming nor a hunter-gatherer lifestyle are considered viable in such circumstances.

The assumed surface conditions reflect the consideration of the relevant processes PG-29 and PG-31 as given in Appendix A.

4.1.4 Biosphere modelling approach

Radionuclides released from the barrier system of a deep geological repository are assumed to enter the biosphere system as dissolved species in groundwater that is discharged from deep aquifers[36]. On entry to the biosphere, they become distributed spatially by a number of transport and accumulation processes. An overview of the key processes taken into account in biosphere modelling is described in the context of the SwiBAC code description in Section 4.3.3.

To calculate dose rates, it is necessary to model the distribution of radionuclides within the biosphere area under consideration and to assess the pathways by which the representative person may become exposed to radiation.

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[35] Agricultural practices with a relatively large impact on the biosphere system, such as construction of dams or the melioration of agricultural land by large relocations of soil, are not considered.

[36] Some radionuclides may also be released from a repository via the gas phase, although this release mode is outside the reference scenario and thus beyond the scope of SGT Stage 2. The same holds for other release scenarios, such as release through repository exhumation or through future human actions.

With respect to time scales, the modelling approach consists of:

- transient (dynamic) modelling of processes with characteristic timescales of at least several years, which are mainly the physical transport processes between individual compartments representing e.g. the soil, aquifer and surface water body, and
- an equilibrium treatment of relatively rapid processes occurring on a timescale of around a year or less.

Compartment modelling approaches are typically used to assess radionuclide distributions in the biosphere following release from a geological repository, as described, for example, in IAEA (2003). Efforts to establish international consensus on issues related to biosphere modelling are ongoing, notably through programmes such as the IAEA's project on Modelling and Data for Radiological Impact Assessments (MODARIA[37]) and the collaborative BIOPROTA project[38]. Recent developments in the context of releases to terrestrial and freshwater biosphere systems include those described in Walke et al. (2013) and Avila et al. (2010).

An overview of the transient and equilibrium elements of the present biosphere modelling approach is given separately in the following paragraphs. More details are presented in the following Sections 4.1.5 and 4.1.6.

Dynamic compartment modelling

As noted above, a terrestrial fresh-water ecosystem used for agricultural production is selected for biosphere modelling. A compartment modelling approach is used to obtain the distribution of radionuclides within such a system. Radionuclides can be present in each compartment as aqueous species in solution or associated with solid materials. It is expected that the environmental concentrations of radionuclides released to the ecosystem will be low, such that system dynamics are not perturbed by their presence and solubility limits are not exceeded. As a consequence, stable isotopes of these radionuclides are not needed for biosphere modelling.

Radionuclides migrate between compartments in solution with fluxes of water and by vertical diffusion, as well as with fluxes of solid materials with which they may be associated. Note that some radionuclides can also be released from the soil in the gas phase (see the description of the treatment of C-14 in Section 4.1.7).

It is assumed that radionuclide concentrations in any given compartment are homogeneous. The assumption of homogeneity can be justified by a number of arguments, including, for example, that radionuclides entering a compartment will be rapidly mixed (on a time scale that is short compared with variations in radionuclide release rates from the geological barrier), or that mixing occurs when radionuclides are extracted from a compartment, e.g. due to grazing livestock or to crop harvesting. In any case, an appropriate selection of the spatial dimensions of the model compartments is needed for the validity of this approach[39].

The compartment model for SGT Stage 2 that is implemented using the SwiBAC code is described in general terms in Section 4.1.5, with mathematical details provided in Section 4.2.1.

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[37] Working Group 6 of the MODARIA programme seeks to develop a common framework for addressing environmental change in long-term safety assessments. http://www-ns.iaea.org/ projects/modaria/.

[38] http://www.bioprota.org/.

[39] Elert et al. (1999) have demonstrated that compartment models can appropriately represent radionuclide behaviour in surface soils. Avila et al. (2010) have explored the importance of discretisation assumptions for a relatively coarse biosphere model and conclude that biosphere dose factors are not particularly sensitive to subsurface discretisation.

Equilibrium treatment of biological processes and exposure pathways

Rapid processes, such as the exchange of radionuclides between water and solid materials, are represented within each compartment by an assumption of equilibrium. Similarly, an equilibrium approach is used to represent biological processes occurring in crops, livestock and humans (including radiation effects), where accumulation and internal transport mechanisms are largely determined by cycles operating on annual or even shorter time scales.

Exposure pathways are assessed in accordance with the ICRP 103 definition of effective dose (ICRP 2007) and defined in terms of:

- the intake of radionuclides with drinking water and foodstuffs,
- the inhalation of airborne radionuclides, and
- exposure due to external irradiation from contaminated environmental media.

These exposure pathways are described in general terms in Section 4.1.6. The corresponding mathematical representations are given in Section 4.2.2.

4.1.5 Dynamic compartment model

General description

The biosphere in a potentially affected area is conceptually divided into the following discrete compartments:

- the rooting zone (top) soil of agricultural land,
- the near-surface (local) aquifer,
- the surface water,
- bed sediments associated with the surface water, and
- intermediate (deep) soil horizons between the aquifer and the rooting zone.

Such a discretisation implies that the same compartment properties, irrigation and/or erosion regimes apply to the entire area. In order to allow for different properties and regimes within the area, the soil compartments (top and deep) can be split into several smaller areas. Each smaller area may then have different soil properties, as well as different irrigation or erosion regimes.

The five types of compartment listed above, along with the ancillary compartments required to model the transport of radionuclides within the model domain, are depicted in Fig. 4-1. The figure also shows the fluxes of water, solid material and radionuclides between compartments; these fluxes are described in more detail in the following paragraphs. The names of the compartments are used in the definition of individual fluxes between compartments. Tab. 4-1 describes each compartment along with the associated nomenclature.

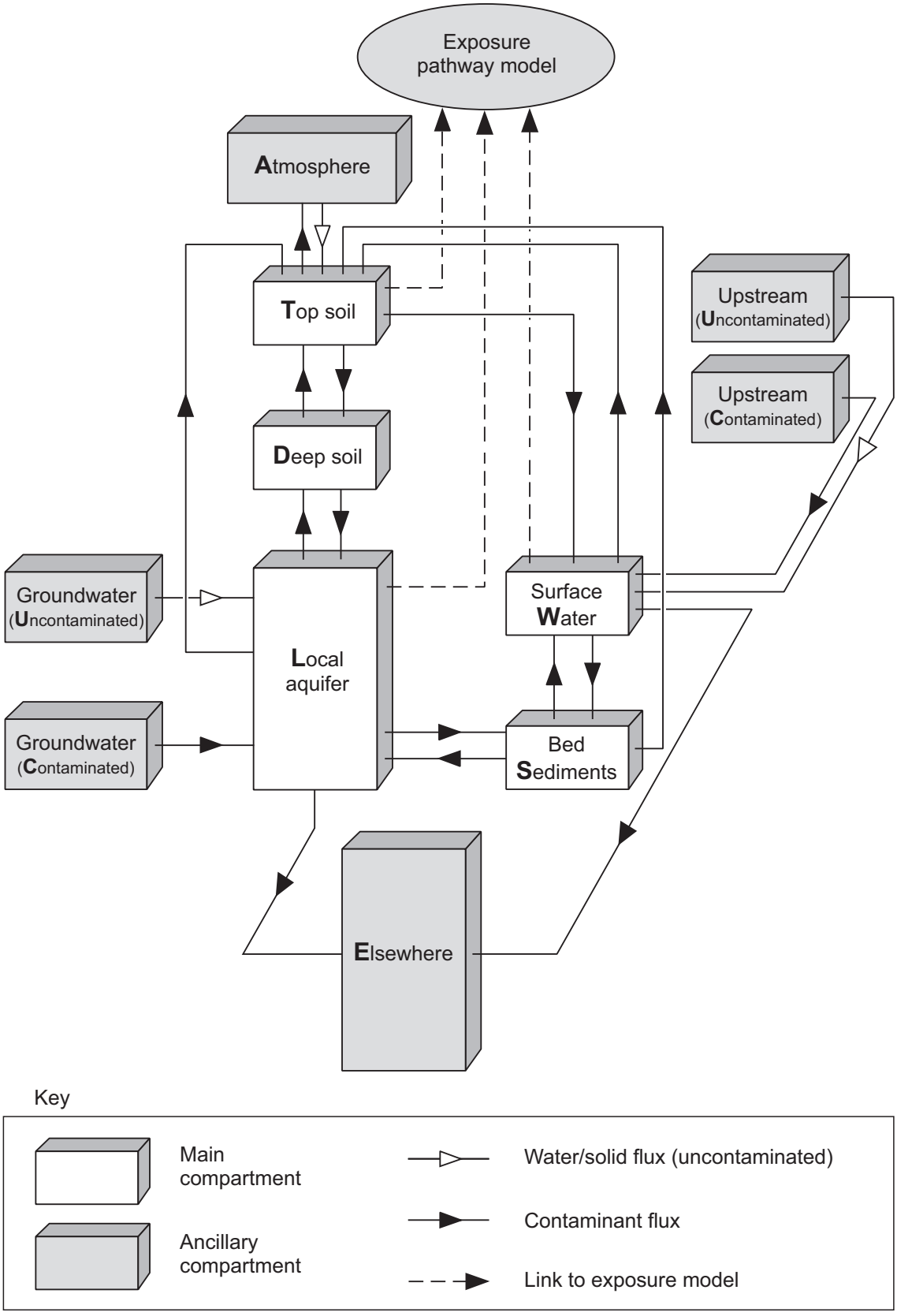

Fig. 4-1: Overview of the dynamic compartment model.
Situation for a model with a single soil area.

Tab. 4-1: Biosphere model compartments and their associated nomenclature.

Compartment	Symbol	Description
Main compartments		
Local Aquifer	L	near-surface geological media supporting groundwater flow, possibly associated with the surface water body
Deep Soil	Dk	soil horizons between the local aquifer and the rooting zone of crops for soil area of index *k*
Top Soil	Tk	soil horizons containing the roots of crops for soil area *k*
Surface Water	W	springs, streams, rivers, ponds, lakes, reservoirs
Aquatic Bed Sediment	S	solid material forming the bed of the surface water body (when distinguished from the aquifer material)
Ancillary compartments		
Contaminated	C	source of contaminated groundwater and suspended solids to the biosphere section
Uncontaminated	U	source of uncontaminated groundwater and suspended solids to the biosphere section
Atmosphere	A	source of uncontaminated precipitation
Elsewhere	E	a compartment acting as a sink for surface run-off and groundwater outflow

Radionuclide source term

In the context of the provisional safety analyses for SGT Stage 2, it is assumed that the transfer from the barrier system of a deep geological repository to the biosphere occurs instantaneously. Transport times between the siting regions and potential discharge areas, dilution / dispersion within the respective deep aquifers, as well as diffusion from the deep aquifers into other low-permeable rock units along this transport path, are omitted.

In reference calculations, the local aquifer is selected to be the recipient compartment for radionuclide releases from the geosphere. This choice is motivated by the following considerations:

- Discharge of deep groundwater in valleys filled with lake sediments is judged unlikely because such sediments are usually fine-grained and thus rather impermeable.
- Discharge into deep gravel layers covered by less permeable layers may result in comparatively long pathways to the surface water bodies, with correspondingly higher radionuclide retention and longer travel times.
- Direct discharge into a river would cause a larger dilution and would thus result in lower individual doses.
- Gaseous release is beyond the scope of the provisional safety analyses in SGT Stage 2.

Water fluxes between compartments

Water fluxes provide one of the means by which radionuclides are transported between compartments. The modelled water fluxes are shown in Fig. 4-2 and the nomenclature is explained in Tab. 4-2.

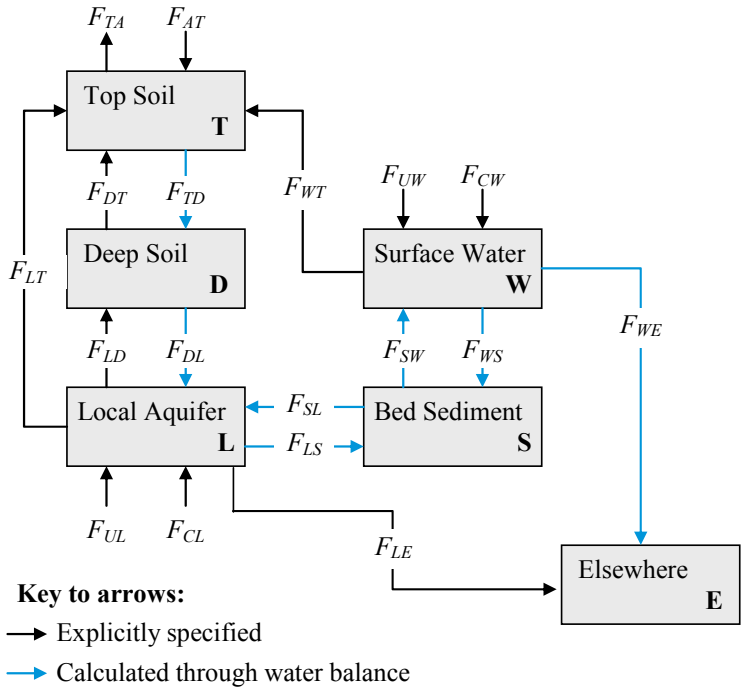

Fig. 4-2: Intercompartmental water fluxes in the dynamic compartment model. Situation for a model with a single soil area.

Tab. 4-2: Nomenclature for water fluxes shown in Fig. 4-2.

Flux	Description
$F_{A,Tk}$	Precipitation for soil area *k*
$F_{Tk,A}$	Evapotranspiration for soil area *k*: evaporation loss to atmosphere (soil/water surface), transpiration loss from plants
$F_{L,Tk}$	Irrigation with groundwater (from local aquifer) for soil area *k*
$F_{W,Tk}$	Flooding and irrigation with surface water for soil area *k*
$F_{Tk,Dk}$	Percolation (infiltration) from top soil to deep soil for soil area *k*
$F_{Dk,Tk}$	Water flux from deep soil to top soil (e.g. capillary rise) for soil area *k*
$F_{Dk,L}$	Percolation (infiltration) from deep soil to local aquifer for soil area *k*
$F_{L,Dk}$	Water flux from local aquifer to deep soil (e.g. capillary rise) for soil area *k*
$F_{U,L}$	Inflow of uncontaminated groundwater into local aquifer
$F_{C,L}$	Discharge of radionuclide-bearing deep groundwater into local aquifer
$F_{L,S}$	Water flux from local aquifer to bed sediments
$F_{S,L}$	Water flux from bed sediments to local aquifer
$F_{S,W}$	Water flux from bed sediments to surface water
$F_{W,S}$	Water flux from surface water to bed sediment
$F_{U,W}$	Flux of uncontaminated water into surface water body (mainly from upstream surface water body, but also precipitation)
$F_{C,W}$	Flux of radionuclide-bearing water into surface water
$F_{W,E}$	Water flux from surface water to sink (out of the model area)
$F_{L,E}$	Water flux from local aquifer to sink (out of the model area)

Solid material fluxes between compartments

Fluxes of radionuclide bearing solid materials provide another means by which radionuclides are transported between compartments. Solid material transport is either connected to water fluxes (e.g. suspended sediment) or is an independent process (e.g. erosion, deposition, bio-turbation). The modelled solid material fluxes are shown in Fig. 4-3 and the nomenclature is explained in Tab. 4-3.

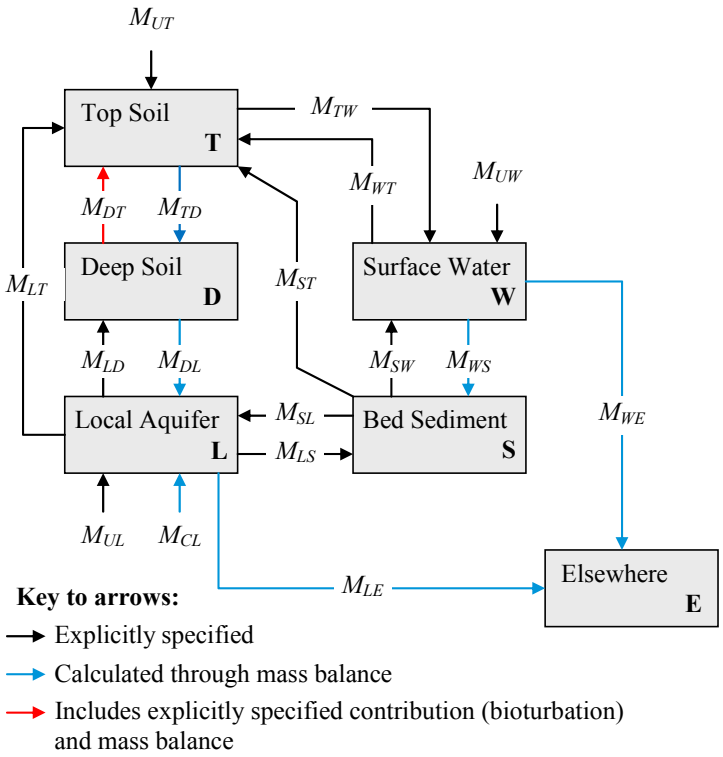

Fig. 4-3: Intercompartmental solid material fluxes in the dynamic compartment model. Situation for a model with a single soil area.

Tab. 4-3: Nomenclature for solid material fluxes shown in Fig. 4-3.

Flux	Description
$M_{L,Tk}$	Solid material flux (suspended solid material) by irrigation with groundwater from local aquifer for soil area k
$M_{W,Tk}$	Solid material flux (suspended solid material) from surface water to top soil by flooding and irrigation for soil area k
$M_{Tk,W}$	Solid material flux from top soil to surface water by erosion for soil area k
$M_{Tk,Dk}$	Solid material flux from top soil to deep soil (e.g. bioturbation and water-mediated transport) for soil area k
$M_{Dk,Tk}$	Solid material flux from deep soil to top soil (e.g. bioturbation) for soil area k
$M_{Dk,L}$	Solid material flux from deep soil to local aquifer (e.g. percolation) for soil area k
$M_{L,Dk}$	Solid material flux from local aquifer to deep soil for soil area k
$M_{U,L}$	Flux of non-radionuclide-bearing solid material into local aquifer
$M_{C,L}$	Balancing flux of uncontaminated solid material into local aquifer
$M_{L,S}$	Solid material flux from local aquifer to bed sediments
$M_{S,L}$	Solid material flux from bed sediments to local aquifer
$M_{L,E}$	Solid material flux from local aquifer to sink (used for mass balance reasons so that dimensions of local aquifer compartment stay constant in case of net deposition)
$M_{W,S}$	Deposition of suspended solid material as bed sediments
$M_{S,W}$	Resuspension of bed sediments
$M_{S,Tk}$	Solid material flux from bed sediment to top soil (e.g. dredging) for soil area k
$M_{U,W}$	Flux of uncontaminated solid material into surface water body (mainly suspended sediment from upstream surface water body) and external deposition on surface water (e.g. from erosion elsewhere)
$M_{U,Tk}$	External deposition on soil surface for soil area k (e.g. from erosion elsewhere)
$M_{W,E}$	Solid material flux from surface water to sink (e.g. suspended sediment and bedload)

Diffusive transfers between compartments

Diffusive transfers operate vertically between the top soil and the deep soil, between the deep soil and the local aquifer and between the local aquifer and the bed sediment, as illustrated in Fig. 4-4. In all other intercompartmental transfers, diffusion processes are not modelled, mainly because the transfer rates are considered negligible with respect to advective / dispersive and solid transfer rates.

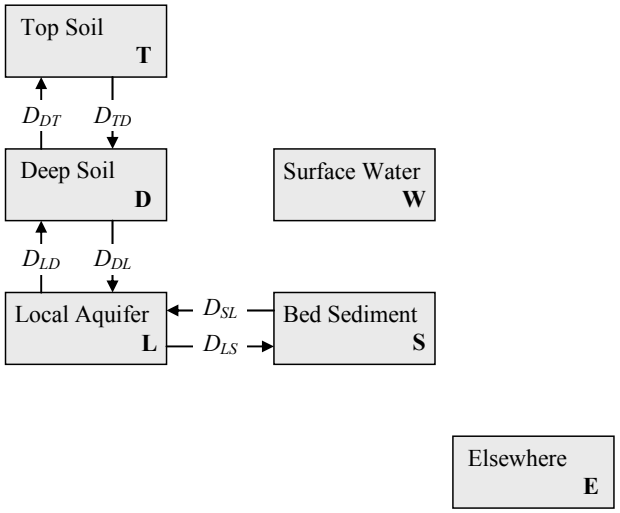

Fig. 4-4: Intercompartmental diffusive transfers in the dynamic compartment model. Situation for a model with a single soil area.

Transport in the gas phase

As noted earlier, some radionuclides can enter the gas phase within the soil. This is of particular importance for C-14, where the exchanges of gaseous carbon between the soil, the plant canopy atmosphere, the plant itself and the atmosphere above the canopy must be taken into account. This is illustrated conceptually in Fig. 4-1 as a transfer to the atmosphere. The modelling of C-14 in the biosphere is described further in Sections 4.1.7 and 4.3.6.

4.1.6 Exposure pathways

The following exposure pathways, shown by red boxes and arrows in Fig. 4-5, are considered:

- Consumption pathways:
  - drinking water,
  - freshwater fish,
  - meat, eggs, milk and dairy products, and
  - grain, green vegetables, root vegetables and fruit.
- Environmental exposures:
  - external irradiation, and
  - inhalation of radioactive dust or radioactive gas having escaped from the top soil.

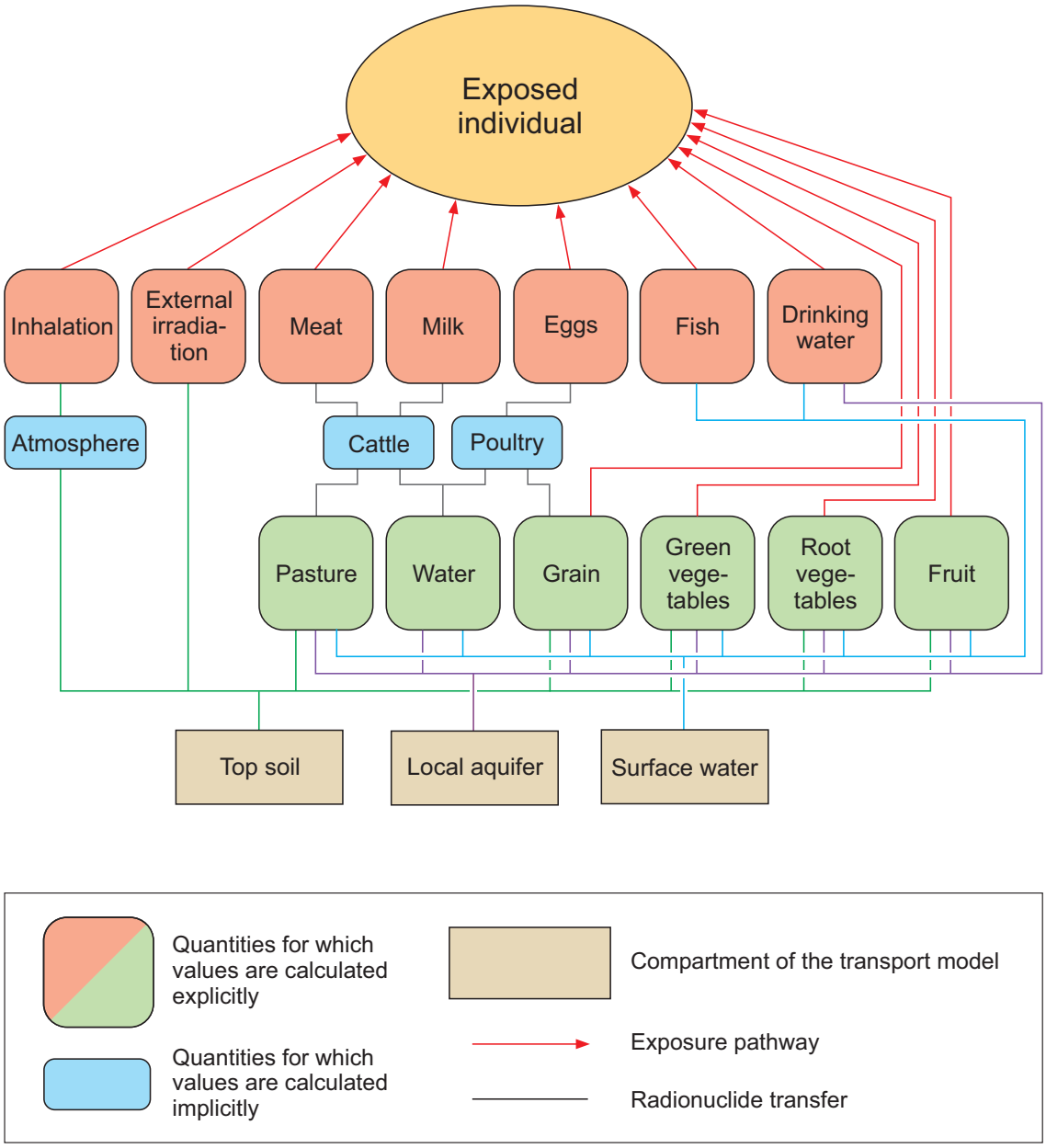

Fig. 4-5: Exposure pathways and the relationship between exposure pathways and the dynamic compartment model.
After Kłos et al. (1996).

These pathways result in potential exposure to radionuclides in one or more compartments of the dynamic compartment model, i.e. in the top soil compartment, in the local aquifer compartment and in the surface water compartment. Note that all radionuclides removed from these compartments by the action of processes in the exposure pathways are conservatively assumed to be recycled annually so that the exposures are not diminished by the pathways acting as external sinks to the dynamic compartment model.

4.1.7 Treatment of C-14

Carbon plays a special role in the biosphere, since it acts as the principal building block of any life form. The dynamics of carbon and its radioactive isotope C-14 in an agricultural biosphere system is thus in some ways different from that of other radionuclides released from the repository. A dynamic transport model tailored to the characteristics of carbon and C-14 is therefore applied. It is implemented in the NC14M v3 code (see Nagra 2013) and summarised in the following paragraphs.

The dynamic transport model for C-14 is conceptually similar to that described in the previous sections for other nuclides, but includes some additional compartments and processes specific to C-14 and stable carbon, including exchange of carbon between the soil, the atmosphere immediately above ground and the higher, more turbulent atmosphere above this. Fundamental assumptions of the transport model for C-14 are that:

- the system is in steady state, such that stable carbon does not accumulate or deplete in the biosphere, and
- photosynthetic isotopic fractionation between C-14 and stable carbon (C-12) is relatively unimportant.

C-14 is taken to behave in the same manner as stable carbon in the biosphere. Therefore, the transport model for C-14 is defined in terms of carbon pools, each represented by a compartment, and the transfers between them (see Fig. 4-6).

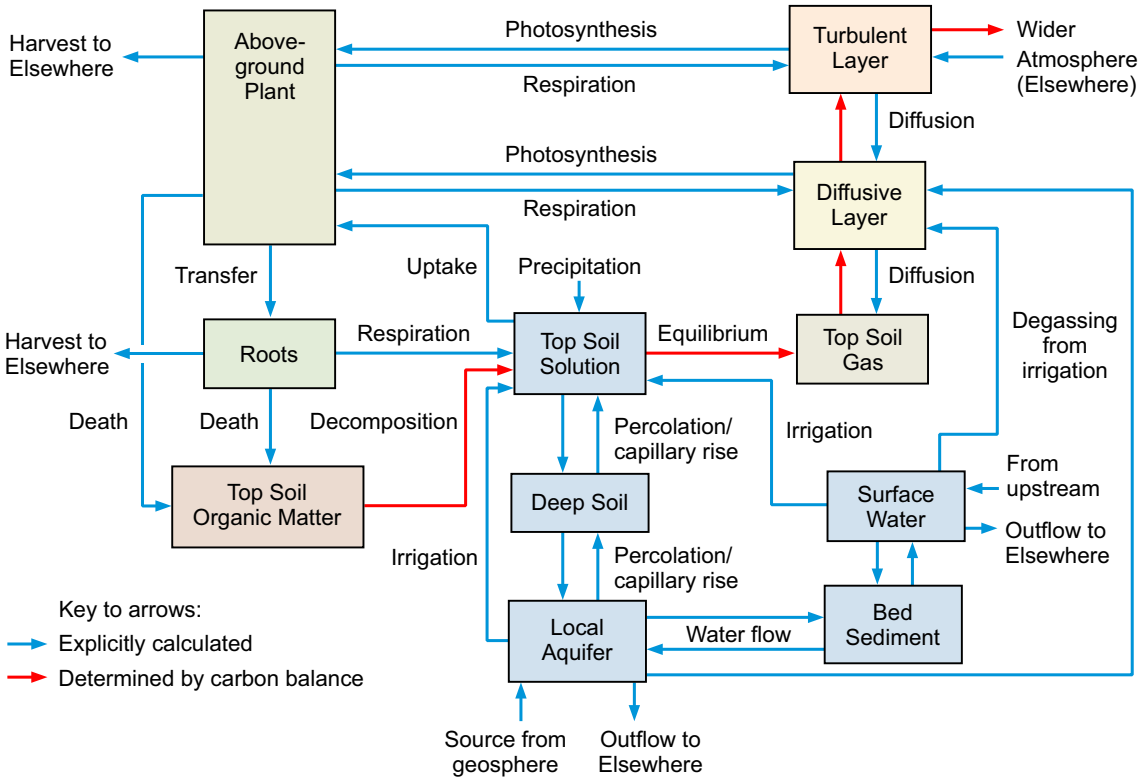

Fig. 4-6: Transfers of stable carbon / C-14 between model compartments.

Transfers are calculated explicitly (blue arrows) or determined by the carbon balance (red arrows). After Figure 2 in Nagra (2013).

The model thus consists of:

- the (time-invariant) amount of stable carbon in each compartment, and
- steady-state fluxes of stable carbon between the compartments.

Transfer rates of C-14 within the biosphere system can then be calculated based on the transfer rates determined for stable carbon. The transfer rates obtained enable the steady-state distribution of C-14 within the biosphere system to be modelled for a given release rate of C-14 from the geosphere.

The model includes release of C-14 from the soil gas to a lower layer of the atmosphere within the plant canopy. Exchange between this lower layer and the higher, more turbulent atmospheric layer is conservatively represented as being diffusion dominated[40]. Advective and diffusive exchanges are then represented between the more turbulent layer and the wider atmosphere, which acts as both a source of stable carbon as well as a sink for C-14 in the gas phase. Plants can take-up C-14 from both the diffusive and turbulent layers of the atmosphere, as well as from the soil solution in the transpiration stream.

As explained in Section 4.3.6, the distribution of C-14 within the biosphere system calculated in this way can be used to determine effective soil-to-plant concentration ratios, effective top soil solid / liquid partitioning coefficients and a loss rate of C-14 due to release to the wider atmosphere and due to losses in harvested crops that have taken up this radionuclide. These effective parameters can then be used in the standard dynamic compartment model, as implemented in the code SwiBAC, to calculate dose rates resulting from the modelled exposure pathways.

4.1.8 Biosphere dose conversion factors

In Section 4.1.1, it was pointed out that the ultimate role of biosphere modelling is to convert potential radionuclide releases from the engineered and geological barrier system into effective dose rates. A key feature of such releases is that – for most radionuclides – they vary over timescales that are much longer than the timescales characterising the most relevant transfer and accumulation processes in the biosphere. This observation leads to the possibility of assuming that an equilibrium exists at any given time between the radionuclide concentrations in the various compartments and thus of calculating steady-state biosphere dose conversion factors (BDCFs) as a convenient way to convert geosphere release rates into dose rates.

Formally, the BDCFs are the radionuclide-specific dose rates at equilibrium arising from a hypothetical, time-invariant constant unit release of a radionuclide from the geosphere. All relevant exposure pathways are taken into account when calculating these dose rates. The use of BDCFs is beneficial from a modelling point of view, since the BDCFs only need to be calculated once for a given biosphere model setup. Transient dose rates can then be conveniently calculated for any number of near-field and geosphere release and transport calculations by multiplying the radionuclide-specific, time-dependent release rates from the geosphere by their respective BDCFs and summing the results over the relevant radionuclides.

The assumption of short response times of radionuclide concentrations in the biosphere relative to changes in the release rates from the engineered and geological barrier system may not be justified for some radionuclides. This is particularly the case for hydrophilic and weakly-sorbing radionuclides, which are likely to accumulate relatively slowly in the top soil (see Brennwald & van Dorp 2008). In these cases, the equilibrium assumption tends to yield pessimistic BDCFs.

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[40] In reality, there will be advection and turbulent mixing within what is shown as the "diffusive layer" in Fig. 4-6. However, its representation as a diffusion-dominated layer is a conservative simplification because it will result in higher CO_2 concentrations and therefore higher C-14 concentrations in the crop.

An important consideration in evaluating BDCFs is the treatment of short-lived progeny within the decay chains. In the near-field and geosphere release and transport calculations, these radionuclides are not calculated explicitly, since they decay to insignificance during transport before reaching the biosphere. However, these short-lived progeny can be significant contributors to dose rates in the biosphere. In order to account for this phenomenon – for each of the exposure modes of ingestion, inhalation and external radiation – the dose coefficients of the short-lived daughters are summed and added to the dose coefficient of their longer-lived parent, taking branching ratios into account. Short-lived radionuclides are taken to be those with half-lives of less than 60 days, which is deemed a reasonable choice considering the fact that the timescales of radionuclide transfer between the biosphere compartments are of the order of years or longer (see Section 4.1.4).

4.2 Mathematical representation

This section provides a brief mathematical description of the biosphere model used for reference calculations in SGT Stage 2 and implemented in the SwiBAC code. It is a summary of the more complete description given in Section 4 of Walke & Keesmann (2013). Further details are provided in Kłos et al. (1996). For mathematical details about the NC14M model, the reader is referred to Nagra (2013).

In the description of the dynamic compartment model given in the previous section, it is pointed out that the soil compartments (Top Soil and Deep Soil) can be split into several separate areas and each soil area may have different properties. The use of multiple soil areas is referred to, where appropriate, in the following, and is implemented in the SwiBAC code as described in Section 4.3.

4.2.1 Evolution of the radionuclide inventory in a compartment

The transport of radionuclides between the main compartments of the biosphere model is modelled based on mass balance considerations. The amount of nuclide N in compartment i is denoted by N_i. The transfer interactions are then denoted by a set of fractional transfer rates λ_{ij} from this compartment to the other j compartments in the system and fractional transfer rates λ_{ji} to this compartment from the others. The rate of change of the content of compartment i is therefore:

$$\frac{\partial N_i}{\partial t} = \left(\sum_{j \neq i} \lambda_{ji} N_j + \sigma_{MN} \lambda_N M_i + S_{N,i} \right) - \left(\sum_{j \neq i} \lambda_{ij} N_i + \lambda_N N_i \right) \qquad (4.2\text{-}1)$$

with

N_j	inventory of nuclide N in compartment j [Bq]
M_i	amount of the precursor radionuclide of N in compartment i [Bq]
λ_{ij}	fractional transfer rate from compartment i to j [T^{-1}]
λ_N	decay constant for radionuclide N [T^{-1}]
σ_{MN}	branching ratio for decay from contaminant M to N [-]
$S_{N,i}$	external source term of radionuclide N into compartment i [Bq T^{-1}].

Radionuclides are transferred between the compartments by water and solid material fluxes. In addition, vertical diffusion processes can also play a role between compartments with differing concentrations. The general form of the coefficients that describe radionuclide transfer is:

$$\lambda_{ij} = \frac{1}{\theta_i + (1-\varepsilon_i)\rho_i K_{d,i}} \left(\frac{F_{ij} + K_{d,i} M_{ij}}{l_i A_i} + D_{ij} \right) \tag{4.2-2}$$

with

F_{ij} water flux from compartment i to compartment j [L^3 T^{-1}]

M_{ij} solid material flux from compartment i to compartment j [M T^{-1}]

D_{ij} effective vertical diffusion rate for dissolved radionuclides diffusing from compartment i to compartment j [T^{-1}].

These are linked to the physical properties of the system:

l_i depth / thickness of compartment i [L]

A_i surface (plan) area of compartment i [L^2]

θ_i volumetric moisture content of compartment i [-]

ε_i porosity of compartment i [-]

ρ_i solid dry density of compartment i [M L^{-3}]

$K_{d,i}$ solid-liquid distribution coefficient for the considered radionuclide in compartment i [L^3 M^{-1}] [-].

Note that, within each compartment, environmental concentrations of radionuclides can be assumed to be at trace levels. It is thus possible to model the equilibrium partitioning of radionuclides between the aqueous phase and the solid phases in a simple way, using the K_d concept (for a detailed discussion about this concept, see Kłos et al. 1996). Radionuclide uptake by plants growing in the top-soil compartment is modelled using empirical soil / plant concentration ratios (see Walke et al. 2013b).

Expressions used for determining specific water and solid material fluxes from the characteristics of the biosphere are given in Sections 4.2.2 and 4.2.3 of Walke & Keesmann (2013), respectively. The intercompartmental water fluxes F_{ij} are related to the relevant process PG-31 in Appendix A.

The effective diffusion rate for dissolved radionuclides from compartment i to compartment j is approximated by:

$$D_{ij} = s_{ij} \cdot \frac{1}{l_i \cdot \min(l_i, l_j)} \cdot \frac{D_0}{T_i} \tag{4.2-3}$$

with

D_0 diffusion coefficient in pure water [L^2 T^{-1}]

T_i compartmental tortuosity [-]

s_{ij} an area scaling factor [-].

The area scaling factor is set to unity, except in cases where the area of interface between two compartments is not the full area of one of the compartments. This applies e.g. to the transfer from the local aquifer (L) to the deep soil (D), when multiple soil areas are used. In that case, the transfer rates for the separate deep soil compartments are scaled by the fraction of the overall area that they represent.

4.2.2 Evaluation of dose via exposure pathways

The dynamic compartment model provides time-dependent inventories of the nuclide N in compartment i as a function of time, $N_i(t)$ [Bq], where the relevant compartments for exposure are top soil, local aquifer and surface water. The annual individual effective dose from exposure to radionuclide N originating from each of these compartments i for exposure pathway p, $D_p^{(N)}(t)$ [Sv T^{-1}], is given by:

$$D_p^{(N)}(t) = \sum_i H_{\text{exp}}^{(N)} \cdot E_p \cdot P_{p,i} \cdot N_i(t) \qquad (4.2\text{-}4)$$

with

$E_p P_{p,i}$ product of E_p, an exposure factor for pathway p, e.g. consumption rate or occupancy, and $P_{p,i}$, a processing factor that converts the inventory, N_i, into a concentration [T^{-1}]

$H_{\text{exp}}^{(N)}$ dose coefficient for radionuclide N and exposure mode "exp" (inhalation, etc.) [Sv Bq^{-1}] (for treatment of short-lived radionuclides, see Section 4.1.8).

Expressions used for determining $E_p P_{p,i}$ for the various exposure pathways are given in Sections 4.3 and 4.4 of Walke & Keesmann (2013).

Where multiple soil areas are included in the model, each crop (including pasture) is assumed to be grown in a particular area and so the relevant top soil compartment is used to calculate the resulting dose rate. External irradiation and dust inhalation are treated by averaging (weighted by area) over all the different top soil areas.

4.3 The SwiBAC code

4.3.1 Scope and purpose

The Nagra biosphere modelling approach is implemented in the Swiss Biosphere Assessment Code, SwiBAC, which supersedes Nagra's earlier biosphere modelling code, TAME (Kłos et al. 1996, Nagra 2002a). The model implemented in SwiBAC Version 1.2 is documented in Walke & Keesmann (2013).

SwiBAC evaluates the distribution of radionuclides in a terrestrial fresh-water ecosystem used for agriculture with the dynamic compartment modelling approach described in the previous sections. It then evaluates potential exposure of humans for the most relevant exposure pathways, using the calculated radionuclide concentrations in the compartments "top soil", "surface water" and "local aquifer". By assuming steady-state conditions, SwiBAC can be used to calculate biosphere dose conversion factors (BDCFs), as defined in Section 4.1.8. Alternatively, the calculation steps outlined above can be repeated for successive time steps to provide, as output, time-varying radionuclide-specific individual effective dose rates.

A specific feature of SwiBAC is that it allows full tracking of radionuclides that enter the biosphere and of those that contribute to the calculated dose rates. This allows the contribution resulting from ingrowth of radioactive progeny occurring in the biosphere to be accounted for in the biosphere dose conversion factor for the parent radionuclide, without the need for multiple calculations.

4.3.2 The model domain

As described in Section 4.1, the biosphere is taken to include the land occupied by the more highly exposed group of humans (as defined in Section 4.1.1), the vegetation, livestock and other fauna also present, the atmosphere and surface waters and, below ground, soils and an underlying near-surface aquifer.

A river section is the basic unit selected for biosphere modelling. Its size depends on the size of the region directly affected by the potential release from the geosphere (typically given by the width of the near-surface aquifer) and / or by the minimum area that is necessary to provide the group of humans under consideration with local products.

In principle, individual river sections can be linked together within SwiBAC to represent a longer river section with spatially varying properties. This facility is, however, not used in the biosphere modelling carried out for SGT Stage 2 and is therefore not described further in the present report.

4.3.3 Processes and parameters

In SwiBAC, radionuclide transfer between compartments occurs by:

- advection of dissolved radionuclides with water fluxes,
- diffusion of dissolved radionuclides between compartments that are vertically adjacent to each other, and / or
- movement of solid material with which radionuclides have become associated between compartments.

Solubility limitation of solute concentrations is not taken into account.

Water fluxes between compartments can be specified directly by the user, taking into account relevant environmental and agricultural processes. Alternatively, some water fluxes can be calculated internally by SwiBAC, based on the processes that drive the fluxes, for which rates are then required as input parameters. These processes include:

- precipitation,
- evapotranspiration,
- irrigation with surface water (including flooding) and with groundwater, and
- capillary rise (including other processes driving water fluxes from the local aquifer to deep soil and from deep soil to top soil).

Water fluxes may carry with them suspensions of solid, radionuclide-bearing materials. The processes taken into account in calculating solid material fluxes include (explicitly or implicitly):

- erosion of soil,
- bioturbation,
- deposition and re-suspension of sediments, and
- dredging of sediments.

SwiBAC calculates human exposure due to consumption of drinking water and of various food-stuffs, external irradiation and inhalation of radioactive dust or gas. In order to calculate the radionuclide content of foodstuffs (meat, milk, eggs, fish, fruit, grain and vegetables), processes implicitly or explicitly taken into account include:

- plant photosynthesis and respiration,
- root uptake,
- translocation (movement of materials from leaves to edible tissues),
- the consumption of soil, plant materials and water by animals,
- respiration of animals and excretion,
- decomposition of plants and animals, and
- food processing.

Kinetic and dynamic processes within the human body, as well as internal exposure mechanisms, are implicitly taken into account by applying the legally binding dose coefficients.

4.3.4 Solution method

The SwiBAC model is implemented in the AMBER general-purpose compartmental modelling tool (Quintessa 2011). The approach adopted is to use an AMBER template file, which holds the structure of the model and all of the expressions required, and to provide athe required input parameter values by substituting placeholders in that template file. The substitution file that contains the required input information is written by SwiBAC once the user input has been parsed and checked. AMBER then undertakes the required calculation and creates various out-put files. These files are processed by SwiBAC and the requested results are returned to the user.

SwiBAC allows the user to select between two solvers built into AMBER: a Laplace solver and a time-step solver. The former is the default when calculating steady-state biosphere dose conversion factors (see Section 4.1.8). The time-step solver must be used when calculating dose rates for geosphere releases read from a file. The user can also choose whether to use SwiBAC to calculate water and solid material fluxes, or to impose these via the input files.

SwiBAC produces a log file and various additional output files. If biosphere dose conversion factors are to be calculated, these are written to an output file. When radionuclides released from the geosphere are read from an input file, two output files are created: one reporting the total dose rate versus time and one giving the contributions to dose rate from each calculated radionuclide. Any other parameter value generated by the AMBER calculation can be written to output files at the request of the user.

4.3.5 Input requirements

The input structure and syntax for SwiBAC are described in a user guide. Standard data, such as lists of radionuclides and decay chains, dose coefficients and data for standard calculations are included as libraries and can be specified as include files. In calculations where dose rates arising from time-dependent geosphere releases are to be assessed, the geosphere release rates are provided as source files with the format of PICNIC-TD input and output files for radionuclide fluxes.

Parameter values given to SwiBAC must have units explicitly stated. The units must be convertible to the code-internal units. The units are specified in the same way as for STMAN and PICNIC-TD. A complete list of input parameters to SwiBAC is given in Walke & Keesmann (2013).

4.3.6 Implementation of the C-14 model and interfacing with SwiBAC

The NC14M compartment model for the treatment of C-14 in biosphere modelling, as described in Section 4.1.7, has also been implemented in the AMBER generic compartment modelling software (Quintessa 2011). The version NC14M v3, as documented in Nagra (2013), is used for the present dose calculations.

The implementation of the C-14 model in AMBER is fully consistent with the SwiBAC water flow assumptions[41]. However, the C-14 model also includes compartments for the representation of the crop plant and the atmosphere, both of which do not exist in the SwiBAC transport model. Moreover, the harvest of the crop and discharges to the wider atmosphere both result in a loss of C-14 from the system. In the standard SwiBAC model, the only losses of radionuclides from the system are the outflow of radionuclides dissolved in water and associated with suspended sediments from the compartments Surface Water and Local Aquifer, as well as radioactive decay. The pathways of ingestion via harvest of crops, use of animal products and drinking water, as well as the pathway of inhalation via degassing from soil, are taken into account in the exposure model, but without impact on the distribution of radionuclides in the system.

The retention of C-14 in SwiBAC has to be made to match the retention of C-14 in NC14M, so that SwiBAC can be used to model C-14 exposure pathways and to calculate dose rates. Thus, an additional C-14 loss term due to harvest and degassing has been introduced into the SwiBAC model, which is, for simplicity, not included in the standard SwiBAC description given in earlier sections. NC14M provides as output effective solid / liquid distribution coefficients for C-14 in the SwiBAC compartments Top Soil, Deep Soil and Local Aquifer and a soil-to-plant concentration ratio for use in SwiBAC[42]. Use of the additional loss term from the top soil, of the effective solid / liquid distribution coefficient and of the soil-to-plant concentration ratios allows SwiBAC to match the retention and soil-to-plant uptake observed in NC14M.

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[41] Transport of C-14 via the solid material and diffusive fluxes in SwiBAC is taken to be relatively unimportant (see Section 2.2 of Nagra 2013).

[42] The derivation of the additional loss term, the effective solid / liquid distribution coefficients and the soil-to-plant concentration ratios is described in detail in Section 3.5 of Nagra (2013).

4.3.7 Verification

Key test cases have been simulated with the earlier version 1.1 of the SwiBAC code and verified against pre-existing simulations. The results are summarised in the following paragraphs.

Recalculation of BCDFs from earlier safety assessments

SwiBAC has been used to re-calculate biosphere dose conversion factors (BDCFs) for a reference biosphere system and for a warmer, drier variant that were originally calculated using Nagra's earlier biosphere modelling code TAME (Kłos et al. 1996), based on concepts and parameters in Nagra (2010b) and in Brennwald & van Dorp (2008).

SwiBAC implements the same transport and exposure models as TAME and so it is expected to give the same BDCFs. Verification results show good agreement between the BDCFs calculated with SwiBAC and TAME, with difference less than 1 % throughout. Minor discrepancies have been noted that could be due to the number of significant digits used in the input, but none are large enough to be important.

The good agreement between the two codes shows, in particular, that:

- the AMBER model is behaving correctly,
- SwiBAC's template files are correct,
- SwiBAC transmits the parameters to AMBER correctly, and
- the results are read back from AMBER correctly.

Transient calculations with constant source

Transient results leading to the steady-state BDCFs are also available from both the SwiBAC calculations (using the time-stepping solver) and the TAME calculations. Fig. 4-7 compares the transient results for a selection of five radionuclides and shows the excellent agreement that is obtained. In a further test, a constant source maintained for 1'000 years was calculated using SwiBAC. The same five radionuclides were used as in the previous test. As shown in Fig. 4-8, the SwiBAC results, as expected, follow the BDCF results of TAME up to 1'000 years and then decrease to zero rapidly for some radionuclides (Cl-36 and Cs-135) and over thousands to tens of thousands of years for others.

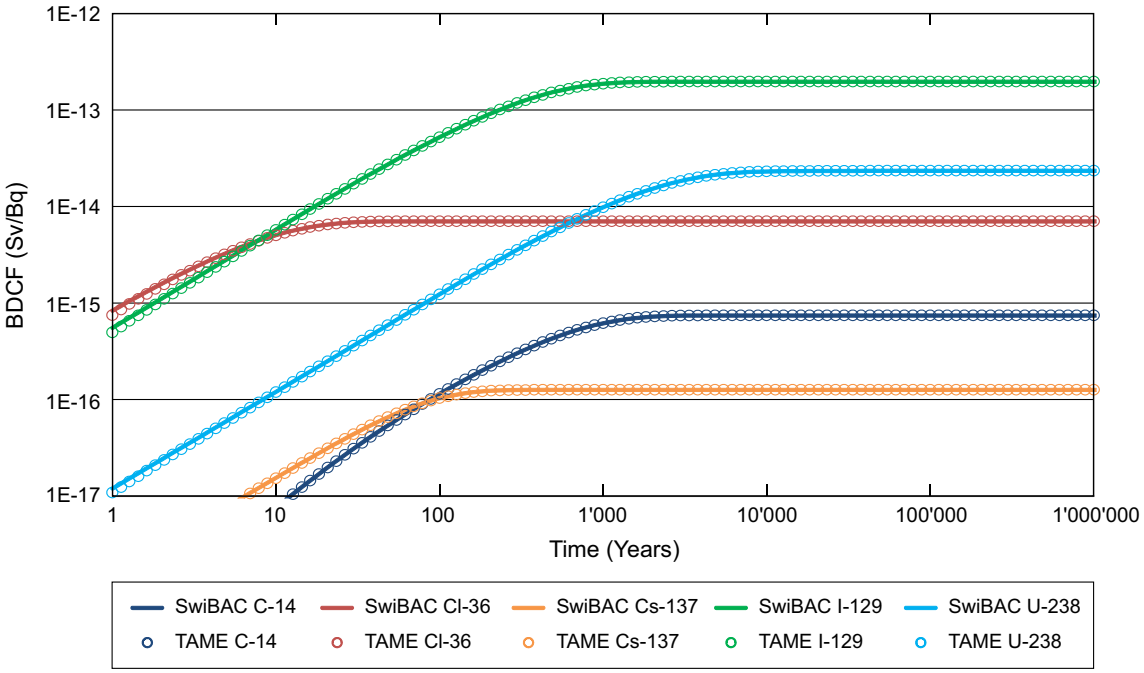

Fig. 4-7: Comparison of transient results for BCDFs for selected radionuclides between SwiBAC and TAME calculations.

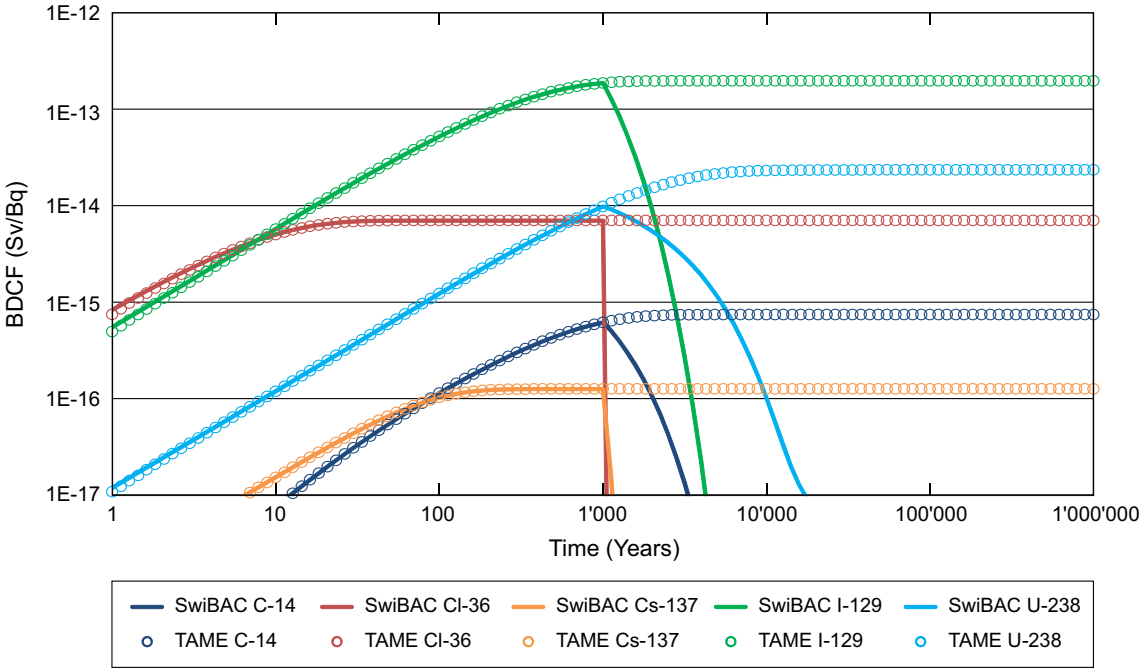

Fig. 4-8: Comparison of transient results for BDCFs for five selected radionuclides with a time-limited constant source.

Realistic PICNIC-TD source term

As a test involving a more complex source term, the output file produced by a PICNIC-TD test involving the Cm-246 decay chain was used. Fig. 4-9 shows that the shapes of the dose curves reflect the shapes of the source fluxes, as expected since the timescales over which the PICNIC-TD release fluxes vary are long compared with the time needed for the biosphere to reach equilibrium (see discussion in Section 4.1.8). The ratios between the peak dose rates and the peak radionuclide fluxes were found to be consistent with the BDCFs.

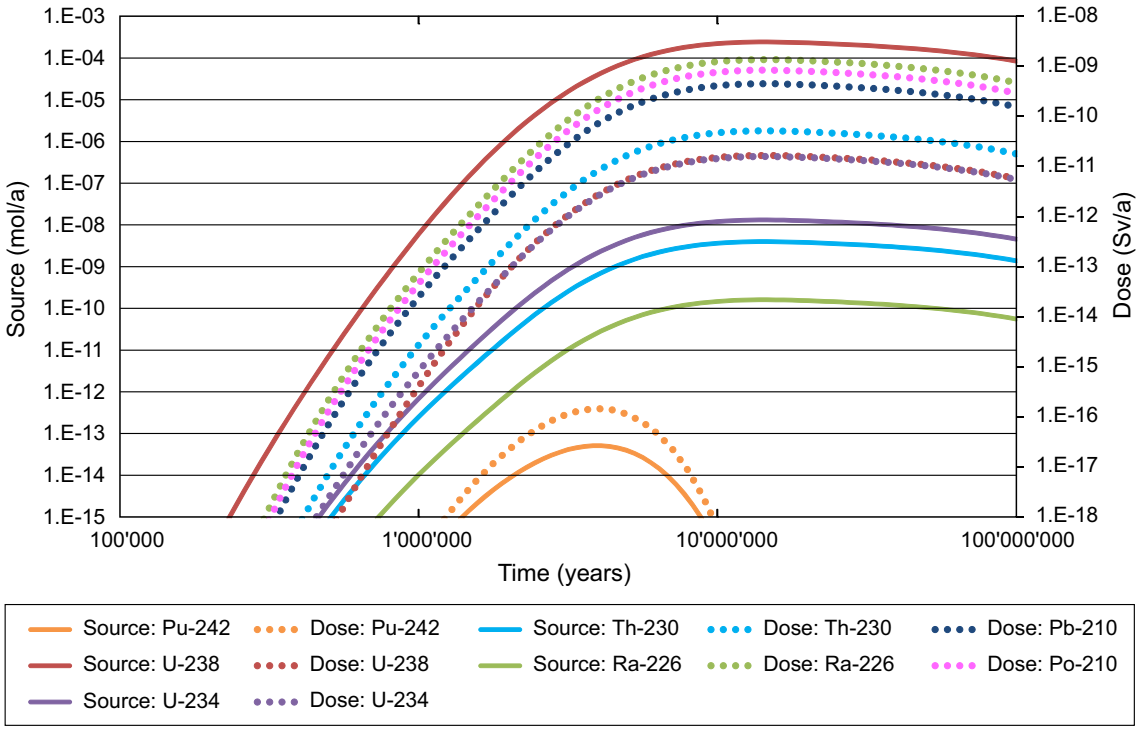

Fig. 4-9: Comparison of SwiBAC dose rate against time-dependent radionuclide source term from PICNIC-TD.

C-14 retention in the top soil compartment

The correctness of the representation of C-14 in the SwiBAC model, as described in Section 4.3.6, has been verified by checking the retention of C-14 in the top soil against that given by the C-14 model reported in Nagra (2013). Fig. 4-10 shows the good long-term agreement between the retention of C-14 in the top soil calculated with SwiBAC and that presented in Nagra (2013). The C-14 model itself, i.e. the NC14M code v3, has also been verified.

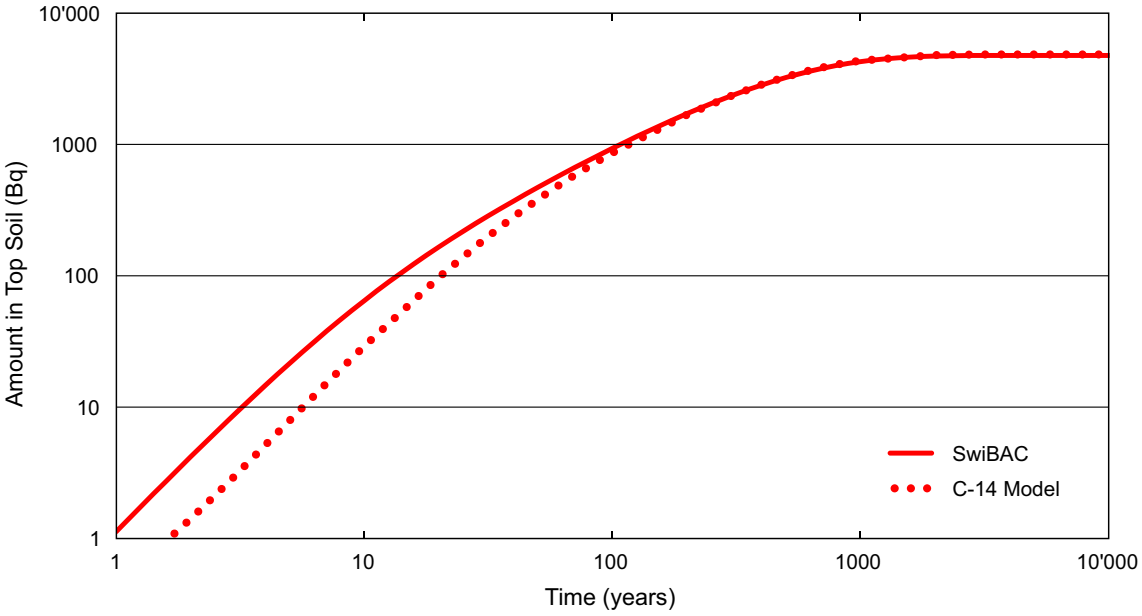

Fig. 4-10: C-14 retention in top soil calculated with SwiBAC compared with that calculated for a generic crop with the C-14 model presented in Nagra (2013).
After Figure 10 of Nagra (2013).

Testing of new capabilities

Some new capabilities have been implemented in SwiBAC version 1.2, mainly aimed at providing increased flexibility in the way in which inputs can be defined. These new capabilities are as follows.

- Translocation of radionuclides adhering to the external surfaces of crops to the edible tissues of these crops can be defined as a fraction (new approach) or as a rate (previous approach).
- Transfer factors from animal feed to eggs can be defined on a mass basis, consistent with most source data, as well as the previous "per egg" basis.

These changes are reflected in additional options available for user input and do not change the underlying models. This has been verified by re-running the full set of test cases used in the verification of SwiBAC 1.1.

5 General Modelling Approach

This chapter describes in detail all aspects of the general modelling approach, which comprises the generic assumptions and parameters needed to model radionuclide release and transport within the engineered and geological barriers. The topics of code selection, code application and code interfacing form an integral part of this discussion. Note that information about the individual calculation cases, including site-specific concepts of radionuclide transport in the geosphere and the corresponding input parameter values, is to be found principally in Nagra (2014b).

The general modelling approach is broadly the same as in SGT Stage 1 (see e.g. Nagra 2008d). However, a more detailed understanding of the geological conditions in the individual geological siting regions, some new capabilities of the safety assessment codes and certain requirements that are specific to the dose calculations in SGT Stage 2 have led to some extensions and modifications.

In Section 5.1, key requirements on radionuclide transport modelling in the framework of the dose calculations are discussed. Section 5.2 defines the system to be modelled. This includes the definition of system boundaries, generic system geometry, types of source terms and types of boundary conditions and initial conditions. Further aspects are the conceptual subdivision of the model system into the near-field model domain and the geosphere model domain, as well as the water flow and solute transport processes considered. Recall that, in the context of the provisional safety analyses for SGT Stage 2, the system to be modelled comprises only the engineered and geological barriers. The biosphere is not considered as part of the barrier system of a deep geological repository (see Chapter 4).

The near-field model domain is explained in more detail in Section 5.3. This section includes exhaustive descriptions of the different types of near-field model and the associated inventory types, of the modelling approaches for nuclide release, water flow and nuclide transport in the different near-field model types, of the coupling between the near field and the geosphere model domains, and of code selection and code application issues.

Section 5.4 describes the geosphere model domain at length. It starts with a description of the different geological elements to be considered in the geosphere models and proceeds with the definition of the source term, with the general modelling approaches for water flow and radionuclide transport in the geosphere and with numerical aspects concerning the selected code.

5.1 Requirements

The general requirements on safety assessment for a deep geological repository are set out in ENSI (2009a). Additional requirements that are specific to the provisional safety analyses in SGT Stage 2 are given in ENSI (2010b) and in ENSI (2013).

In Section 1.1, it is pointed out that the results of the provisional safety analyses provide input to the safety-related comparison of the geological siting regions in SGT Stage 2. This implies that the dose calculations, as part of the provisional safety analyses, should be carried out, as far as reasonably possible, in a realistic manner in order to obtain a comparison that is unbiased in favour of any of the geological siting regions.

At the same time, a further objective of the provisional safety analyses is to show that the calculated individual effective dose rates are below the regulatory protection criterion 1 of 0.1 mSv/a. It follows that the respective dose calculations should not be based on concepts and data that underestimate radiological consequences. Given that there are inevitably uncertainties in the characteristics and evolution of the barrier systems to be analysed[43], some conservative assumptions and pessimistic parameter values aimed at clearly overestimating radiological consequences are therefore unavoidable.

Based on these considerations, the following additional requirements have been established for nuclide release and transport modelling in the framework of the dose calculations for the provisional safety analyses in SGT Stage 2:

1. Results to be compared (i.e. results for the same repository type or the same part of a repository type) must be based on the same general modelling approach and be calculated with the same set of codes.[44]
2. Modelling approaches and parameter values that are likely to underestimate radiological consequences should be avoided.[45]
3. Case-specific modelling approaches should be consistent with the general modelling approach.
4. Highly conservative modelling approaches and parameter values should be avoided, as these may mask prevailing differences between the geological siting regions.

[43] Uncertainties also arise from modelling itself, e.g. due to conceptual uncertainties in the selected modelling approaches.

[44] For instance, dose calculations for the L/ILW repository are all carried out with the same near-field code, even if differences between host rocks would otherwise imply that alternative codes could be used.

[45] If it is a priori not clear which conceptual assumption / parameter value yields the least favourable results in terms of dose, a set of bounding situations may be analysed (see ENSI 2013).

5.2 Model system definition

The model system definition may be summarised in four key statements, each of which is presented below in boxes, and explained in detail in the main text.

1. The horizontal extent of the model system is limited to the individual emplacement areas of a deep geological repository (SF/HLW emplacement area, ILW emplacement area and / or L/ILW emplacement area). Each emplacement area is composed of a number of emplacement rooms, which are assumed to be identical, parallel and evenly spaced horizontal structures, resulting in the emplacement areas that are rectangular in shape. The individual radioactive waste packages and waste types are not assigned to a particular location within an emplacement area or emplacement room. Rather, average inventories are assigned to all disposal canisters or waste packages containing a given waste type or group of waste types.

The model system is tailored to the release scenario to be investigated, which is the release of dissolved radionuclides along the groundwater pathway under the premise that the engineered barriers function correctly. This means, in particular, that no radionuclide transport along the underground structures of a geological repository needs to be considered in the context of the present dose calculations. Therefore, the horizontal extent of the model system is limited to the individual emplacement areas of a deep geological repository.[46] Thus, in the case of the HLW repository, there are two separate emplacement areas to be modelled, one for ILW and one for SF / HLW. In the case of the L/ILW repository, there is a single emplacement area to be modelled. A combined repository system would comprise all three types of emplacement area.

The pilot facility, in which a relatively small but representative amount of the radioactive waste will be emplaced, is not modelled as separate emplacement area. Rather, its nuclide inventory is added to the inventory of the main facility. The final layout and dimensions of the emplacement areas will only be defined during their construction, since these will to some extent be adapted to geological conditions as they are encountered underground. Thus, for SGT Stage 2, a simple and generic geometry of the emplacement areas is assumed, as illustrated in Fig. 5-1.

The modelled emplacement areas are rectangular and horizontal. The emplacement rooms within each emplacement area are identical, parallel and evenly spaced structures that meet the boundaries of the emplacement area at right angles. The emplacement rooms have length L and separation distance d. Thus, the total size of the emplacement area is $L \cdot W$, where W is the product of d and n, n being the number of emplacement rooms within the emplacement area. The dimensions of the modelled emplacement areas in the context of the present dose calculations are given in Nagra (2014b). Individual emplacement rooms within the SF/HLW emplacement area may contain disposal canisters for SF and / or disposal canisters for HLW. In the case of ILW and L/ILW, separate emplacement rooms will be provided for different waste groups. Waste groups are collections of different waste types with similar impact on barrier efficiency in the near field (see Section 5.3.2).

[46] Here, it is implicitly assumed that the individual emplacement areas do also not interact physically or chemically with each other.

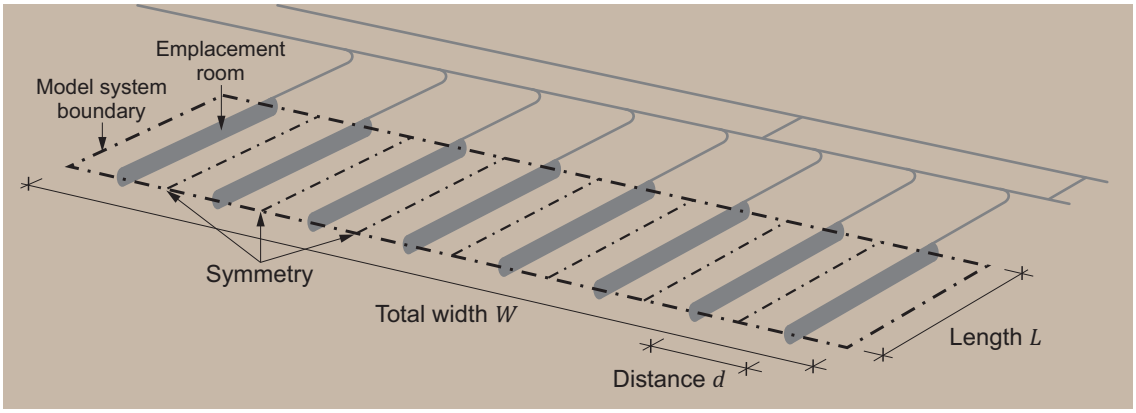

Fig. 5-1: Illustration of an emplacement area with simplified geometry and an idealised arrangement of the individual emplacement rooms.

Waste with average inventory is assumed to be homogeneously distributed across all emplacement rooms within the emplacement area. Symmetry refers to symmetry in the patterns of water flow and solute transport under the assumption of no water flow and no solute transport across the model system boundary.

As noted above, the final layout and dimensions of the emplacement areas will only be defined during their construction. Furthermore, the locations of individual waste packages and waste types within these areas will probably be defined later during the repository operational phase. Therefore, in the context of the on-going site-selection process, the individual radioactive waste canisters, packages and waste groups are not assigned a particular location within an emplacement area or emplacement room. Rather, average inventories are assigned to all disposal canisters or waste packages containing a given waste type or group of types.[47] Nuclide release and transport from the emplacement rooms and their immediate environment are, however, modelled separately for each waste type or waste group, and the calculated releases to the host rock are superimposed.

In the reference case, there is assumed to be neither water flow nor solute transport across the lateral model system boundary depicted in Fig. 5-1. This assumption allows the exploitation of symmetries within and between the emplacement rooms in setting the boundaries for the nuclide release and transport calculations in the emplacement rooms and their immediate environment (see Section 5.3.1).

[47] This is consistent with the approach that, for each waste sort, which is a collection of waste types with similar characteristics, the average nuclide inventory is used for the dose calculations (see Section 5.3.2).

2. The modelled volume around each emplacement area extends above and below the repository horizon to include the low permeable effective containment zone (ECZ). The extent of the ECZ may be specific to any given geological situation, depending on the barrier efficiency of individual transport paths within the host rock and / or the confining units. In the reference case, no water flow and nuclide transport occurs across the lateral boundaries of the ECZ. The top and bottom boundaries of the ECZ are release points from the model system. Radionuclides that arrive at these release points are assumed to be immediately transferred to the same biosphere. The modelled volume is conceptually split into two model domains: the near field and the geosphere, which are modelled consecutively. The different rock units[48] of the ECZ are mostly conceptualised as horizontally bedded homogeneous porous media (with the exception of certain rock units interspersed with joints or faults). Thus, in the reference case, groundwater flow and solute transport in the geosphere are both one-dimensional and vertically orientated.

The modelled volume around the emplacement areas extends above and below the repository horizon to include the geological formations that substantially contribute to the effective containment of any radionuclides released from the disposed waste (see Fig. 5-2). This part of the geological environment is termed effective containment zone (ECZ).[49] The extent of the ECZ may be specific to any given geological situation, depending on the barrier efficiency of individual transport paths within the host rock formation and / or the confining units. The part of the host rock formation that has the most favourable confinement properties and that is large enough to host the repository is termed host rock in its strict sense. Each emplacement area has associated with it a single ECZ with specific geological properties.[50]

The lateral boundaries of the modelled part of the ECZ are defined by the horizontal extent of its associated emplacement area, as illustrated in Fig. 5-1. In the reference case, no water flow and nuclide transport occurs across the lateral boundaries of the ECZ.[51] Fixed values for the hydraulic head are applied at the top and bottom boundaries of the ECZ. The nuclide concentrations at these boundaries are set to zero. Thus, nuclides released from the emplacement rooms and arriving at these boundaries can escape from the model system. The top and bottom boundaries are therefore called release points (even though they may have significant lateral extent). Radionuclides arriving at the release points are modelled as being transferred instantaneously and completely to the same biosphere system.

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48 In Nagra (2014b), the term "lithofacial unit" is used for a given part of the geosphere that is assumed to have homogeneous properties. In this report, the term "rock unit" is used as a synonym.

49 In German: "Einschlusswirksamer Gebirgsbereich (EG)".

50 Note that the geological properties may differ between the emplacement areas of a combined repository system for HLW and L/ILW.

51 The reference scenario assumes that the emplacement rooms are properly sealed so that horizontal water flow and transport of dissolved radionuclides along the repository tunnel system are negligible. Transport inside the SF/HLW emplacement rooms is prevented through the construction of intermediate seals. The hypothetical effects of ineffective seals on radionuclide transport in solution are analysed in Nagra (2014c). An alternative modelling approach for radionuclide transport across the side boundaries of the modelled domain along localised water-bearing tectonic-structural elements is described in Section 5.4.3.

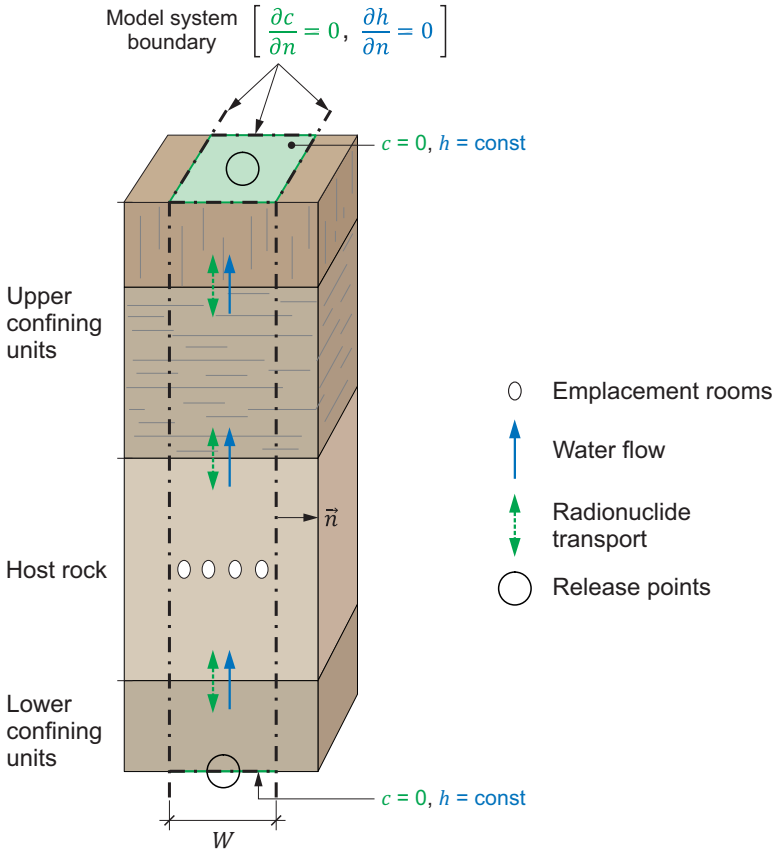

Fig. 5-2: Schematic illustration of the model domain associated with a given emplacement area and a given geological situation.

The modelled volume around each emplacement area is split into two model domains:

- The near field comprises a single L/ILW emplacement room, a single ILW emplacement room or a single SF / HLW disposal canister (including the backfill material around it), as well as the immediate geological environment around these features.[52]
- The geosphere covers those parts of the ECZ that are physically and chemically unaffected, or only marginally affected, by the presence of the repository during the modelling period, i.e. after the period of complete containment.

Each domain of the model system is modelled individually and with specific codes, while respecting the requirements outlined in the previous section.

Near-field release and transport modelling is carried out first and provides, as output, radionuclide release rates to the geosphere. The total near-field release rate from an emplacement area is obtained by summation over the near-field release rates from all corresponding near-field models. Next, geosphere transport modelling is carried out using, as input, the calculated total near-field release rates of radionuclides[53] and providing, as output, radionuclide release rates

[52] Note that for each calculation case, the flow and transport parameter values of the immediate geological environment of the emplacement rooms in the near-field domain are chosen to be consistent with the parameter values in the corresponding model for the geosphere domain.

[53] In this report, the more general term *nuclide* is usually used. However, if the context involves decay or ingrowth of nuclides or discusses the radiological hazard of the waste in general, then the term *radionuclide* is preferred.

from the effective containment zone of the emplacement area under study. The total release rate from the barrier system of a deep geological repository is obtained by summing over the geosphere release rates from the ECZs associated with all individual emplacement areas of the repository. The total radionuclide release rate from the barrier system is converted into an individual effective dose rate by multiplying the radionuclide-specific release rates by their corresponding biosphere dose conversion factors (BCDFs), which are calculated using the biosphere model (see Section 4.1.8), and then summing over all calculated radionuclides. The set of codes used, and the information flows between them, forms what is also called the model chain (see Fig. 2-2).

For the purpose of the dose calculations, it is assumed that the rock formations that constitute the ECZ are horizontal and that they display no lateral (i.e. horizontal) variability in water flow and solute transport properties. Hence, groundwater flow and radionuclide transport occur on average perpendicularly to its top and bottom boundaries, i.e. in vertical direction. Since the emplacement areas are also assumed to be horizontal, water flow through the emplacement rooms is on average vertical (see e.g. Fig. 5-3), although, for L/ILW and ILW, some limited horizontal flow may occur in the vicinity of any transmissive geological elements intersecting the emplacement caverns.[54]

The geosphere part of the ECZ is conceptualised for modelling purposes as a vertical stack of rock units. Each rock unit differs from those adjacent to it in its water flow and solute transport properties (e.g. because it has a distinct rock mineralogy). The rock units are modelled either as homogeneous porous media or as uniformly fractured porous media. In the latter case, the fractures are assumed to be parallel, vertical planar features. Anisotropy in the water flow and solute transport properties of a rock unit can occur mainly due to its bedding, so that differences in hydraulic conductivity and diffusion coefficients in the vertical and horizontal directions may need to be accounted for. Consistently with the simplifications concerning the uniform distribution of the different waste types within an emplacement area and the use of average nuclide inventories (see above), transport of radionuclides in the geosphere is modelled broadly as a one-dimensional, vertical process (though with horizontal matrix diffusion in rock units modelled as uniformly fractured media).

3. The concepts for modelling nuclide release and transport in the near field and for modelling radionuclide transport in the geosphere incorporate the processes that are most relevant to radionuclide release from the barrier system. Water flow and solute transport are assumed to occur under water-saturated conditions.

As described in Chapter 3, the generic concepts for modelling nuclide release and transport in the near field and for modelling radionuclide transport in the geosphere incorporate the processes that are most relevant to radionuclide release from the barrier system along the groundwater pathway. The model representations of these processes also presented in Chapter 3 are considered to be well supported by current scientific understanding.

Furthermore, the term radionuclide is also used for the geosphere model domain, since stable nuclides are not considered in geosphere transport calculations.

[54] The assumption of average vertical flow through the emplacement caverns may not be fully consistent with the hydrogeological situation in some of the geological siting regions for the L/ILW repository, where groundwater flow through the emplacement caverns is possibly oblique (see Nagra 2014b). However, with respect to other conceptual and parametric uncertainties, oblique water flow through L/ILW emplacement caverns has generally only a minor influence on calculated near-field release rates, as has been shown in the course of SGT Stage 1 for a broad range of hydrogeological situations, including situations where faults intersect the L/ILW emplacement caverns (Nagra 2008c).

The processes considered explicitly in the context of the dose calculations are:

- radionuclide decay and ingrowth,
- instant and / or gradual release of nuclides (radionuclides and stable isotopes) from the waste matrices to solution,
- saturated groundwater flow, along with advective / dispersive and diffusive transport of radionuclides and stable isotopes in solution, and
- reversible immobilisation of nuclides due to sorption on solid particles and / or due to precipitation.[55]

The same pessimistic containment time is generally assumed for all waste canisters or packages of the same type (e.g. for all SF / HLW disposal canisters). The assumption of simultaneous loss of containment is conservative, in that it results in the superposition of the peak release rates from all affected canisters or packages. It is further generally assumed that the void space of all porous materials present in the barrier systems is fully water-saturated over the modelling period. This implies that all nuclides released from the waste forms are in the form of distinct, mobile aqueous chemical species, except when sorbed or precipitated (see Section 3.1).

In reality, there is the possibility of partial desaturation in the repository near field, e.g. due to gas generation and accumulation. For the given reference scenario, this has the favourable effect of delaying or slowing advective and diffusive transport in the aqueous phase. However, there may be other effects on the transport of dissolved nuclides through the barrier system, the consequences of which are discussed in Nagra (2014b) with references to other specific reports.

4. The modelling period for nuclide release and transport in the barrier system extends from the end of the period of complete containment to 10 million years. During the modelling period, constant conditions reflecting a stable geological environment are assumed in the reference case.

Nuclide release and transport starts at the end of the period of complete containment, the duration of which may vary between waste types. Prior to this time, only the processes of radioactive decay and ingrowth are modelled.

Repository-induced phenomena, e.g. the desaturation of parts of the host rock during construction and operation, the possible convergence of the emplacement rooms after repository closure or the dissipation of heat resulting from the residual thermal output of SF and HLW are assumed to have diminished to a negligible level by the end of the period of complete containment. Furthermore, the geological siting regions have been selected in part because of the long-term stability of the geological environment. Therefore, nearly all physical and chemical properties of the barrier systems (with the exception of the assessed nuclide concentrations), are assumed to be constant from the end of complete containment until the end of the respective time frames for safety assessment (see Section 1.2).[56] For specific calculation cases, there are however exceptions to this assumption, which are described in Sections 5.3.4 and 5.4.4.

The modelling period is extended to 10 million years after closure, i.e. well above the safety-relevant time frames for the HLW and L/ILW repositories (see Section 1.2), with the aim of better understanding the safety performance and effectiveness of the different barriers at the end

[55] Note that the process of precipitation is disregarded in the geosphere domain since only trace amounts of radionuclides are expected in the geosphere. This assumption results in a mathematically linear system, thus allowing the results of different geosphere models to be superimposed.

[56] For instance, no change in porosity as a result of mineral transformations is taken into account.

of the respective safety-relevant time frames. In performing the analyses, it is hypothetically assumed that the conditions in the barrier systems at the end of the respective safety-relevant time frames prevail up to the end of the modelling period, even though the evolution of the repository barriers is subject to considerable and increasing uncertainties at such times.

5.3 Near field

5.3.1 Description of domain

L/ILW

The L/ILW near-field model domain comprises

- the concrete emplacement containers filled with the radioactive waste,
- the cementitious backfill of the emplacement caverns,
- the construction concrete and the cavern lining, and
- a part of the surrounding host rock.

For the purpose of the present dose calculations, it is assumed that the first three components form a single, cementitious, homogeneous porous medium with isotropic water flow and solute transport properties.[57] The host rock is modelled as a homogeneous porous medium. The reason for including a part of the surrounding host rock in the L/ILW near-field domain is to obtain satisfactory estimates of radionuclide releases across the interface between the engineered structures and the host rock, since it is the low permeable host rock that controls the rate of nuclide release from the emplacement room. A schematic description of the L/ILW near-field model domain is shown in Fig. 5-3.

The current repository concepts provide for some flexibility with respect to the size and shape of the L/ILW emplacement cavern to account for the geological conditions present at a given site (see Section 1.2). For the present dose calculations, two types of L/ILW caverns are used. For a host rock in its strict sense that has a comparatively large vertical extent, a medium sized cavern of type K09 is assumed. It has a width of about 10 m and a height of about 13 m. For host rocks in the strict sense of smaller vertical extent, a smaller cavern of type K04 with a width of about 7 m and a height of about 10 m is assumed.

The excavation of the L/ILW emplacement cavern and the subsequent operational phase will disturb the host rock in the vicinity of the cavern. This disturbance may be due to thermal, hydraulic, mechanical and / or chemical influences. The most relevant and persistent effect for post-closure safety is judged to be the mechanical disturbance, which may result in hydraulic properties of the host rock around the emplacement cavern that are significantly different from those of the undisturbed rock. This disturbed region is referred to as the excavation damage zone (EDZ).

In the L/ILW near-field model, the EDZ is not modelled explicitly for three reasons:

- The thickness of the EDZ will be small compared with the size of the cavern. Furthermore, the cavern can be assumed to be hydraulically highly conductive. Hence, the perturbation of the flow field in the host rock due to the combined presence of the cavern and EDZ, is largely determined by the size and shape of the cavern, even if the EDZ is also assumed to be highly conductive.

[57] The detailed material inventory and distribution in an L/ILW cavern is not explicitly accounted for in the model, but is considered in the derivation of the water flow and solute transport parameters for the cavern (e.g. gaps between emplacement containers provide for a relatively high average hydraulic conductivity).

- Solute transport across the EDZ is of little importance for overall radionuclide release in view of the much larger subsequent transport path lengths in the undisturbed host rock.[58]
- Solute transport along the EDZ, i.e. along the emplacement room, is negligible in light of the assumed high solute transport capacity of the cavern itself.

Convergence of the L/ILW emplacement caverns is expected to be small after backfilling and (partial) resaturation of the near field, due to the strength of the aggregates in the cementitious backfill material (see Nagra 2002b). Thus, the initial dimensions of the selected emplacement cavern types are those considered in the L/ILW near-field models (see Fig. 5-3).

The candidate host rocks in the geological siting regions for the L/ILW repository have a broad spectrum of water flow and solute transport properties, with solute transport regimes that range from mainly diffusive to more advectively influenced, although the advective / dispersive transport capacity is low in all cases. For some host rocks, transmissive elements (e.g. joints and faults) intersecting the emplacement caverns may be relevant. In calculation cases where no transmissive elements intersecting the caverns are considered, 2D modelling of the L/ILW near field is considered to be adequate.[59] If the host rock shows a pattern of densely spaced joints, these are not explicitly accounted for in the near-field model and 2D modelling is also applied, using equivalent water flow and solute transport parameters (see Section 5.3.6). Calculation cases that require the modelling of large transmissive elements (faults) intersecting with the caverns are carried out using a detailed 3D model (see Section 5.3.6).

Making use of the inherent symmetries in the assumed layout and loading of the emplacement areas and emplacement caverns (see Section 5.2), and in the absence of any large transmissive elements intersecting with the caverns, the L/ILW near-field model extends laterally from the vertical plane running along the axis in the middle of an emplacement cavern to the vertical plane at mid-distance to the next cavern (see Fig. 5-3).

Faults intersecting the cavern are assumed to be vertical, parallel and planar structures, with their strike lines running normal to the cavern axis (see Fig. 5-10). The extent of the near-field model in direction of the cavern axis is in this case set to the half distance between two adjacent faults (see also Fig. 5-7). The fault itself is modelled as an equivalent porous medium, but with distinct hydraulic and solute transport properties (for details see Section 5.3.6). For some candidate host rocks for the L/ILW repository, there is the possibility that a tectonic-structural element may exist that conveys water in the horizontal direction. The most unfavourable case would be, if such an element intersected an L/ILW emplacement cavern. To model such a case, another 3D model is used, details of which are also given in Section 5.3.6.

In the vertical direction, the L/ILW near-field model domain extends 50 m upwards and downwards from the centre of the emplacement cavern. The choice of this value is motivated by the minimum requirement for the thickness of the potential effective containment zone in SGT Stage 1 (100 m, see Nagra 2008b). From a modelling point of view, this is seen as an adequate compromise between the two conflicting requirements of (i) setting the boundaries at sufficient distance from the location where near-field release is evaluated (the red dashed line in Fig. 5-3), and of (ii) respecting the influence of release points at the top and at the bottom of the effective containment zone on near-field release.[60]

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[58] However, the EDZ is accounted for in the geosphere model, resulting in shortened transport path lengths through the undisturbed host rock and / or site-specific transport parameter values for the geosphere (see Nagra 2014b).

[59] Since L/ILW caverns are much longer than they are wide (see Section 1.2), three-dimensional water flow and solute transport phenomena at the ends of the caverns can be disregarded.

[60] For individual calculation cases in Nagra (2014b), there are release points as near as 20 m from the centre of the L/ILW emplacement caverns. Test calculations have shown that a distance of 50 m between the model boundary and the caverns is still sufficient for an accurate calculation of near-field release in such cases.

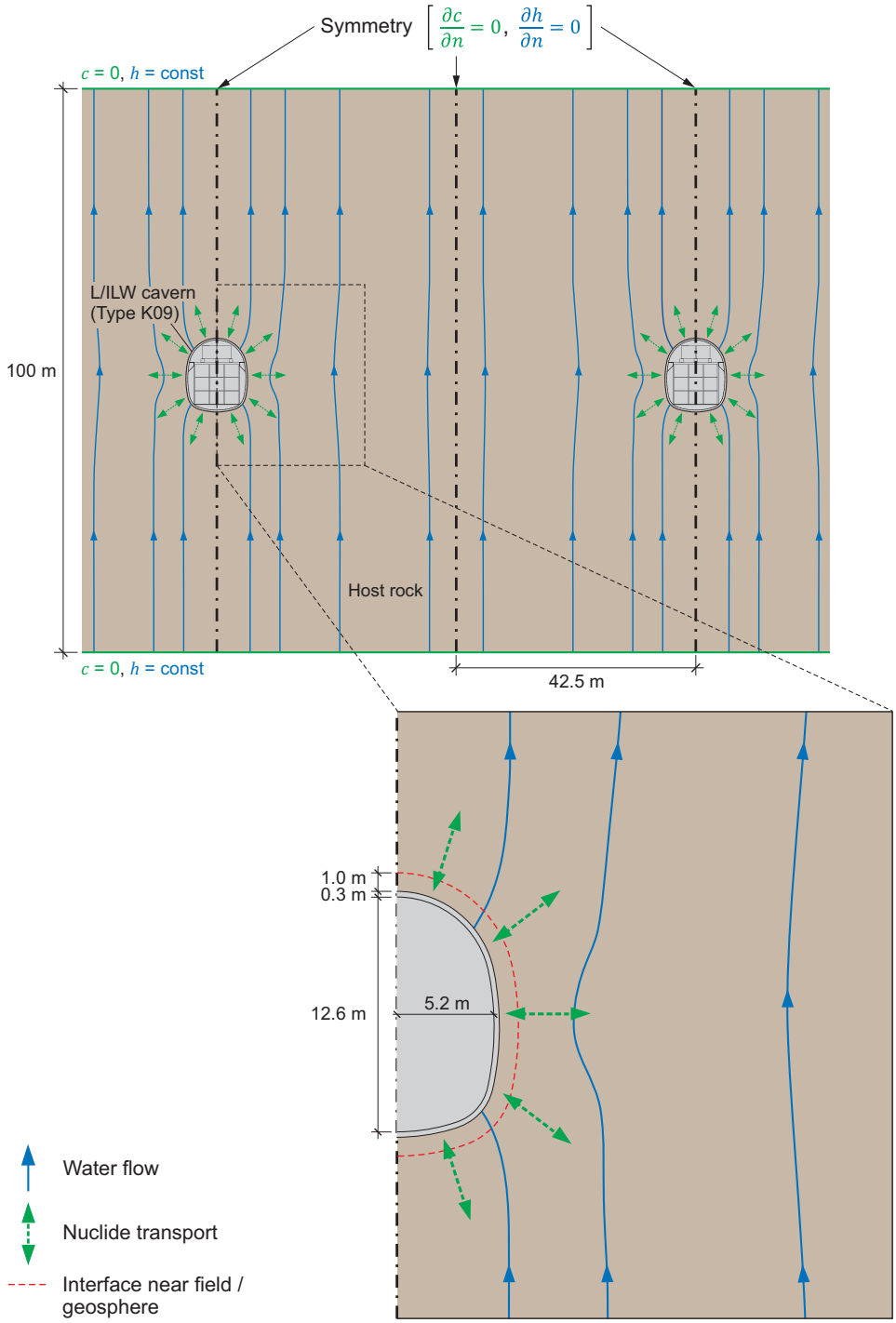

Fig. 5-3: Schematic illustration of water flow and solute transport phenomena in the L/ILW near field based on the cavern type K09 (upper figure) and general modelling approach adopted (lower figure).

For comparison, the height of the alternative cavern type K04 is 9.5 m and its half-width is 3.7 m. Note, that the assumed cavern spacing of 85 m is not fully consistent with the spacing of 100 m assumed for geosphere modelling. However, these differences are jugded to be small with respect to the calculated near-field release rates.

ILW

The ILW near-field model domain comprises, as does the near-field model domain for L/ILW, the concrete emplacement containers with the radioactive waste, the cementitious backfill of the emplacement rooms, the construction concrete, the tunnel lining and a part of the surrounding host rock. Except for the host rock, all components are modelled as a single cementitious homogeneous porous medium with isotropic water flow and solute transport properties. The reason for including a part of the surrounding host rock in the near-field domain is the same as for the L/ILW near-field model domain (see above). A schematic description of the ILW near-field model domain is shown in Fig. 5-4.

With respect to the size and shape of the ILW emplacement room, the situation is similar to the L/ILW emplacement cavern: the influence on near-field release is minor. However, given the geotechnical properties of the Opalinus Clay host rock, the range of possible cavern types is restricted to those with smaller diameters. For the present dose calculations, a small cavern of type K04 with a width of about 7 m and a height of about 10 m, is selected for ILW near-field models. The EDZ around the cavern is not modelled explicitly for the same reasons as in the L/ILW case. Furthermore, the initial dimensions of the ILW emplacement room are those used as the basis for the ILW near-field model, in view of the limited degree of convergence expected.

Due to the very low hydraulic conductivity of the Opalinus Clay host rock, to the expected absence of discrete water-conducting tectonic-structural elements intersecting with the ILW emplacement rooms, and to the expected relatively high diffusive transport capacity of the backfill, nuclide concentrations in the rooms will, to a first approximation, be uniform and radial diffusion into the host rock is expected to be the main near-field release process. The ILW emplacement rooms can therefore be approximated using cylindrical geometry.[61] To this end, the almost elliptical cross-section of the ILW emplacement room of type K04 (58 m^2 cross-sectional area) is represented in the ILW near-field model as a circular cylinder, with the same cross-sectional area as the actual room.

Further away from the ILW emplacement room, nuclide transport in the host rock is more adequately described as a 1D vertical transport phenomenon because of the position of the release points on the top and the bottom of the associated ECZ (see also Kosakowski 2004). Therefore, a hybrid modelling approach is adopted, in which the emplacement room is modelled with a cylindrical geometry and the host rock is modelled using a linear geometry (see Fig. 5-4). This hybrid approach is a special feature of the STMAN code and is described in more detail in Section 3.4.3.

The host rock part of the model, with linear geometry, is connected at its upstream end to the outer boundary of the inner cylinder. To correctly model the diffusive transport capacity of the host rock at the interface between the two parts of the model, the width of the host rock part must be made equal to the circumference of the cylinder. The length of the host rock part of the model is set to 50 m, i.e. to the same distance that the L/ILW near-field model domain extends in both vertical directions (see above).

[61] Although the ILW emplacement caverns may be relatively short and three-dimensional water flow and solute transport phenomena may have a marked effect, the use of cylindrical geometry is judged to be adequate in light of other uncertainties.

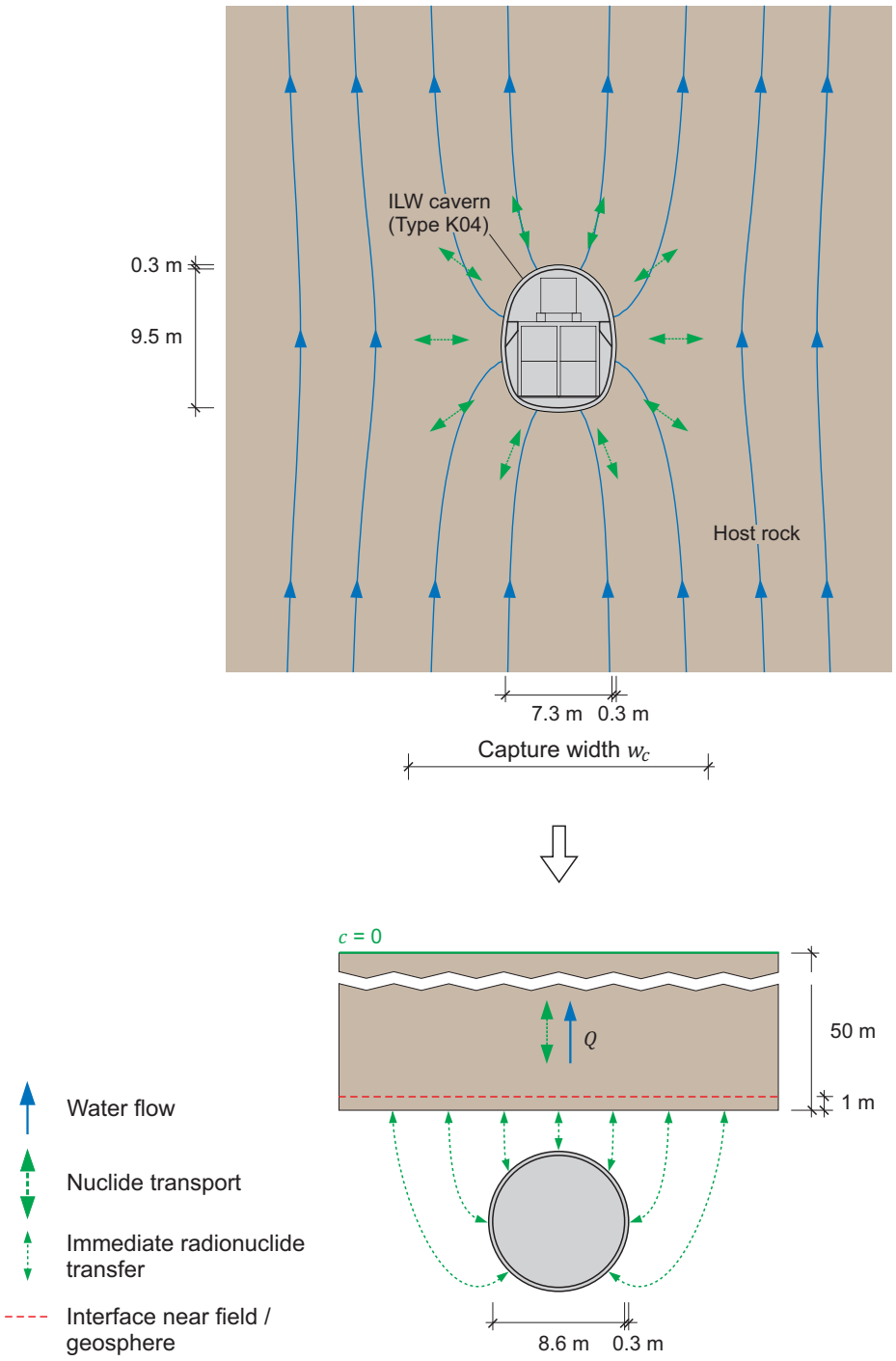

Fig. 5-4: Schematic illustration of water flow and solute transport phenomena in the ILW near field (upper figure) and general modelling approach adopted (lower figure).

SF / HLW

The individual SF and HLW near-field model domains comprise

- a single disposal canister with the respective radioactive waste,
- the surrounding bentonite buffer, and
- a part of the surrounding host rock.

As in the case of other waste types, the reason for including a part of the surrounding host rock in the near-field domain is to obtain satisfactory estimates of radionuclide releases across the interface between the engineered structures and the host rock (see above).

The axial length of the SF / HLW near-field model domain is set to the length of the respective disposal canister type, plus the assumed canister spacing of 3 m. Any intermediate seals present within the SF/HLW emplacement rooms are not explicitly included in the near-field model, but are considered when justifying the assumption that there is no significant transport along the tunnel liner and the EDZ (see below). A schematic illustration of the SF / HLW near-field model domains is shown in Fig. 5-5.

As described in Section 3.2, the void space inside a disposal canister is assumed to become instantaneously saturated when the canister is breaching. The water within this void space is conceptualised as a thin water film (reservoir) in contact with the inner surface of the bentonite buffer. Nuclides are released from the waste forms to this reservoir, and are assumed to have a uniform concentration within it.[62]

The bentonite buffer is modelled as a homogeneous porous medium with isotropic solute transport properties. Chemical interactions between the tunnel liner and the bentonite buffer, as well as between the (corroded) disposal canister and the bentonite buffer, may lead to mineral alterations in the bentonite in the vicinity of both contact surfaces. Furthermore, mineral alterations may also occur due to thermal effects. These possible alterations are addressed by defining separate annular buffer regions adjacent to these surfaces, each with transport parameter values that can vary from those of the unaltered buffer (see Nagra 2014b).

The SF/HLW tunnel liner itself is not modelled as a distinct material class for two reasons:

- its retention capacity is judged to be rather small when compared with those of the (unaltered parts of the) bentonite buffer and of the host rock,
- solute transport along the liner does not need to be considered due to the planned construction of intermediate seals at intervals along the emplacement rooms and due to the assumption of a homogeneously distributed average inventory within the SF/HLW emplacement room.

The second argument is also used to justify the omission of the EDZ around the SF/HLW emplacement room from the SF / HLW near-field models.

There may be some mineral alteration in the Opalinus Clay host rock at its interface with the tunnel due to interaction with the degradation products of cementitious and ferrous materials used for tunnel reinforcement. Its impact on nuclide release and transport is, however, assumed to be negligible in view of the fact that any altered zone will be small compared with the transport path lengths in the undisturbed host rock.

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[62] No credit is taken for transport resistances experienced by nuclides migrating through the canister interior (including, for example, the transport resistances of cracks within the fuel pellets).

Due to the very low hydraulic conductivity of Opalinus Clay and to the expected absence of discrete water-conducting tectonic-structural elements intersecting the SF/HLW emplacement rooms, nuclide transport within the emplacement rooms and its immediate environment will be dominated by diffusion. Modelling the reservoir as an annular feature between the outer boundary of the waste form and the inner boundary of the bentonite buffer, disregarding any residual transport resistance form the breached canister and also disregarding axial diffusion in the space between the disposal canisters, the SF / HLW near field can be modelled with cylindrical geometry.

Further away from the SF / HLW emplacement rooms, nuclide transport is more adequately described as a 1D vertical transport phenomenon, because of the position of the release points on the top and the bottom of the associated ECZ (see also Kosakowski 2004). Therefore, as in the case of ILW, a hybrid approach is adopted in which the emplacement room is modelled with a cylindrical geometry and the host rock is modelled using a linear geometry (see Fig. 5-5). This hybrid approach is a special feature of the STMAN code and is described in more detail in Section 3.4.3.

As in the case of ILW, the host rock part of the model, with linear geometry, is connected at its upstream end to the outer boundary of the inner cylinder. To correctly model the diffusive transport capacity of the host rock at the interface between the two parts of the model, the width of the host rock part must be made equal to the circumference of the cylinder. The length of the host rock part of the model is again set to 50 m, which is consistent with the representation of the host rock in the ILW and L/ILW near-field model domains.

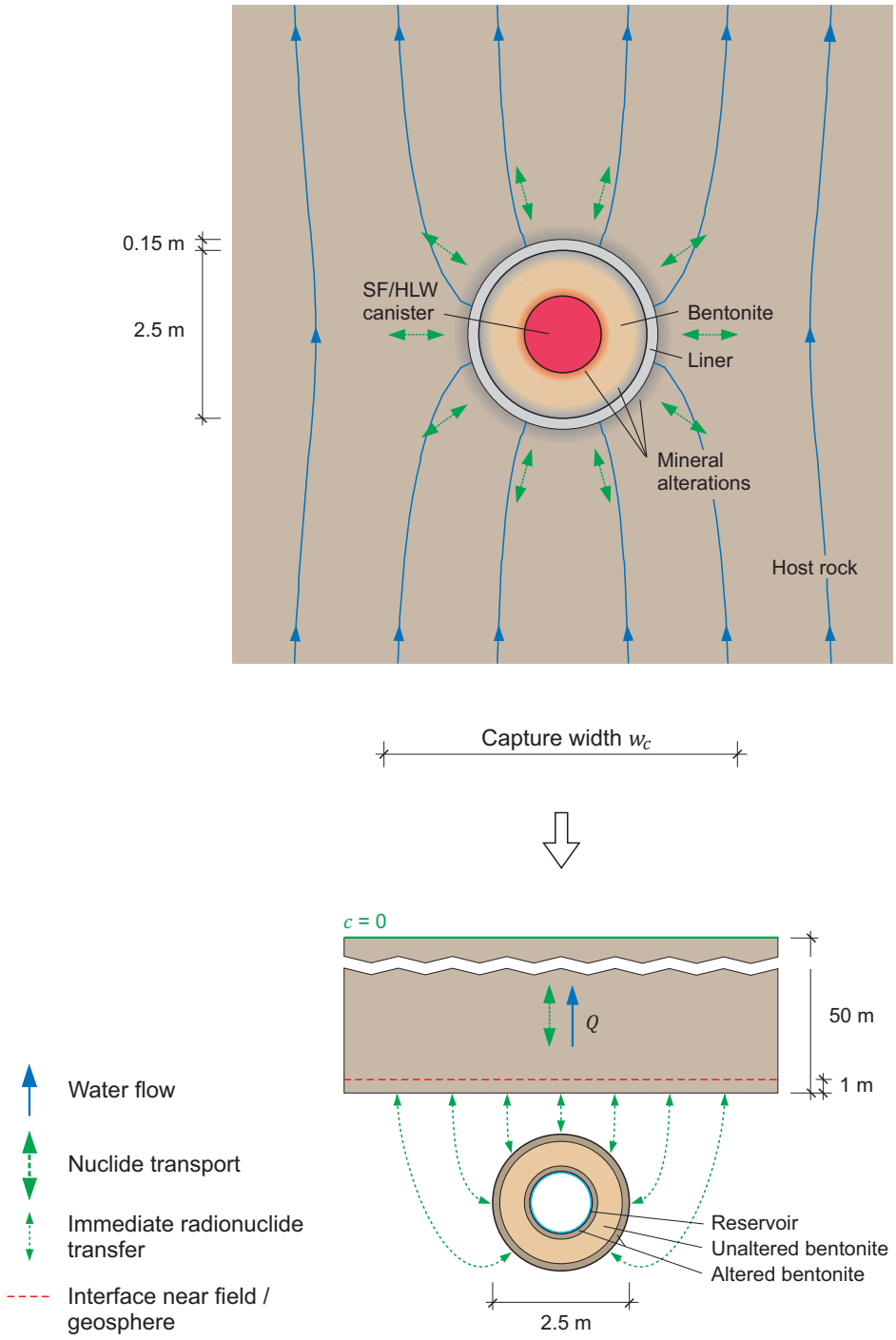

Fig. 5-5: Schematic illustration of water flow and solute transport phenomena in the SF / HLW near field (upper figure) and the general modelling approach adopted (lower figure).

5.3.2 Nuclide inventory and release

General

The modelled inventory of Swiss radioactive materials (MIRAM) is taken as a basis for the dose calculations. An overview of the current MIRAM 14 database is given in the main report (Nagra 2014b).

In MIRAM, the existing and the estimated future radioactive waste packages are grouped hierarchically. At the uppermost level of this hierarchy are waste sorts[63], which may be regarded as model waste packages representative of groups of similar waste packages. Each waste sort belongs to one of the following waste categories: high-level waste, low-level waste or alpha-toxic waste. For each waste sort, average and upper limit values of the amount of radioactive nuclides present are provided. For stable nuclides, best-estimate values are given.

The radionuclide inventories of the different waste sorts are calculated for a reference point in time t_0, which, in the dose calculations, is assumed to coincide with repository closure and hence with the start of the time frames for safety assessment. It is also assumed that waste emplacement, backfilling and sealing of the emplacement rooms occurs simultaneously and instantaneously at this reference point in time.

The low-level and alpha-toxic waste sorts are allocated to the L/ILW repository or to the ILW caverns of the HLW repository based on long-term safety criteria, as described in (Nagra 2014b). In addition, these waste sorts are also subdivided into two different waste groups, depending on their content of materials that may have adverse effects on radionuclide retention in the near field. Overall, four different near-field models are needed for these wastes: two to cover the waste groups allocated to the ILW caverns of the HLW repository (abbreviated ILW-1 and ILW-2), and two to cover the waste groups allocated to the L/ILW repository (L/ILW-1 and L/ILW-2).

To model the near field of the SF/HLW emplacement rooms, the waste sorts, which consist of different fuel assembly (FA) types and different types of flask for HLW, are grouped together as a number of disposal canister types with average properties. There are three types of SF disposal canister and two types of HLW disposal canister, each with specific average nuclide inventories and dimensions. Therefore, five different near-field models for SF / HLW are needed.

Radioactive and stable nuclides that are relevant to the present dose calculations are identified for the SF, the HLW and for the ILW part of the HLW repository, as well as for the L/ILW repository (see Nagra 2014b).

The relevant nuclides are released from the solid waste matrices into the aqueous phase as ions or incorporated in more complex chemical molecules. Whatever the chemical form, it is generally assumed that each nuclide makes up an individual component of the aqueous solution. The specific environmental conditions may affect the chemical form of a nuclide (speciation). From a modelling point of view, this is generally reflected in the assumption of solute transport properties that are specific to the environmental conditions under consideration.

A single speciation is generally assumed for all isotopes of a given chemical element. However, in the particular case of carbon, organic and inorganic forms are modelled as two independent species. In the models and in the results, organic and inorganic carbon are denoted by the symbols *Ch* and *C*, respectively.

The onset of nuclide release to solution may be delayed by some sort of containment, e.g. by an initially tight disposal canister. After loss of containment, e.g. due to the breaching of such a

[63] In German: "Abfallsorten".

canister, water comes into contact with the waste materials and nuclide release starts (mobilisation). A fraction of the nuclide inventory may then be released instantly (called the instant release inventory); the remainder is considered to be released gradually (see Section 3.2).

L/ILW and ILW

In the L/ILW and ILW near-field models, nuclide release starts after a prescribed short containment period of 100 years, which is chosen to reflect the time needed to saturate the respective near fields to the extent necessary for nuclide mobility.[64] In the model, the source terms are uniformly distributed across the entire emplacement rooms. For simplicity, this also includes the cavern lining (see Figs. 5-3 and 5-4). Nuclide mobilisation is modelled by an instantaneous and complete release of the nuclides in the waste packages to solution, while respecting linear sorption equilibrium and solubility limitation (below). As an exception, that part of the C-14 inventory that is associated with massive metallic waste components is assumed to be released congruently as organic species with metal corrosion at a constant rate.[65]

If solubility limits are exceeded, a precipitated phase forms. Solubility limits are potentially exceeded in case of Co, Ni, Sr and inorganic C, since relatively large amounts of stable isotopes of these elements are present in the cement pore water and in the hardened cement paste. Note that, in the L/ILW near-field model, the process of precipitation and redissolution of these elements is approximated by linear sorption equilibrium[66] for computational reasons, whereas, in the case of ILW, precipitation and redissolution are modelled explicity using the approach described in Section 3.2.9. In the ILW near field, the possibility of solubility limits being exceeded is also considered for other elements with relevant stable isotopes that are released from the waste itself.[67]

As explained in Section 5.3.1, a cementitious environment is assumed for the entirety of the L/ILW and ILW emplacement rooms. This means that the specific retention properties of bitumen, polystyrene and other waste conditioning materials are not considered. All other barrier effects, e.g. from the different waste matrices or from different types of containment, are omitted from the near-field models. Furthermore, no credit is taken from any nuclide retention by container materials or their degradation products.

SF / HLW

The release of radionuclides and stable isotopes from the SF and HLW waste forms begins when the disposal canister eventually breaches, e.g. due to mechanical loads, following some degree of weakening by corrosion. In theory, canister breaching may occur locally (e.g. due to the presence of initial penetrating defects) or a larger-scale failure may occur (e.g. due to uniform corrosion). In the present dose calculations, it is assumed that, following breaching, the canister no longer provides any additional physical barrier to water ingress and nuclide release.

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64 It is conservative to assume the same containment period for all waste packages, since the peak release rates due to rapidly released nuclides are then superimposed. The actual containment period is likely to vary between waste packages, so the overall peak release rates, summed over packages, will in reality be lower than those calculated by the near-field models. The containment period is also subject to both aleatory and epistemic uncertainties. Note that, if a probability were to be assigned to the loss of containment at any given time (from one or all packages) based on these uncertainties, and the resulting consequences were calculated in terms of risk, then the phenomenon of risk dilution could arise whereby the higher the uncertainty is estimated to be, the more spread out in time (and hence the lower) is the peak risk (see Wilmot & Robinson 2004).

65 As for instant release, the same duration of congruent release is conservatively adopted for all such waste types.

66 For details on this approach, see Wieland (2014).

67 This refers, in particular, to the inventory of actinides present in alpha-toxic waste.

Furthermore, no credit is taken from any nuclide retention by the disposal canister, the HLW fabrication flask or their corrosion products.

All canisters are conservatively assumed to be breached simultaneously. No credit is taken for the integrity of either the SF Zircaloy cladding (i.e. breaching of the cladding is assumed to occur either before, or immediately upon, canister failure, even though the Zircaloy corrosion rate is expected to be low) or the HLW fabrication flasks.

The initial partitioning of the nuclide inventory associated with spent fuel is discussed in Johnson (2013) and summarised in qualitative terms in Tab. 5-1. Unlike earlier Nagra safety assessments, all carbon originating from the spent fuel matrix is assumed to be in organic form. This assumption is based on (i) the finding in Johnson (2013) that there is currently no sound basis for identifying the chemical form (organic vs. inorganic) of the released C-14, and (ii) the fact that organic carbon is assigned less favourable geosphere diffusion and sorption properties than inorganic carbon (see Nagra 2014b), and hence the assumption of organic carbon is conservative. All carbon originating from the Zircaloy cladding and other structural materials is also conservatively assumed to be released in organic form.

Tab. 5-1: Partitioning and release of SF nuclide inventory (after Johnson 2013).

Spent fuel matrix	**Fuel grain boundaries, cracks in the spent fuel matrix and gaps between the fuel pellets and the cladding**	**Zircaloy cladding and other structural materials**
The nuclides in this part of the inventory are assumed to be uniformly distributed within the SF matrices. They are released congruently as the spent fuel matrices dissolve in water that enters the breached disposal canisters (i.e. water in the reservoir).	This part of the inventory is assumed to be released instantaneously to the reservoir.	Most nuclides in this part of the inventory are assumed to be uniformly distributed within these materials. They are thus, for the most part, assumed to be released congruently as the structural materials corrode at a constant rate. However, a part of the carbon inventory initially present in the cladding is assumed to be released instantaneously.

Fractional matrix dissolution rates and initial instant release fractions (IRFs) for each fuel assembly type are given in Johnson (2013). Values for each SF canister type, required for near-field modelling, are derived by weighted averaging, based on average fuel assembly loading of the canister types under consideration. Since only single nuclides are attributed an IRF in Johnson (2013), the IRF values are taken to be independent of time (see Section 3.2.2).

No partitioning of nuclides is expected for vitrified HLW. The rate of HLW dissolution per unit surface area of wetted glass is assumed to be constant. At production, during cooling of the HLW glass, cracks may have formed, so that the total surface area of the glass fragments at the time of emplacement is greater than that of the original moulded blocks (see Section 3.2.3). The glass fragments are conceptualised as a number of equally sized spheres, with a total volume equal to the total volume of glass and a total surface area equal to the estimated total surface of all glass fragments. Because the surface area of the spheres decreases with time as the glass dissolves, the rate of HLW glass dissolution, and hence the fractional nuclide release rate, also decreases with time.

5.3.3 Water flow and solute transport

L/ILW

Fixed head values are set at the upper and lower boundaries of the L/ILW near-field model. These are chosen to reproduce the average vertical groundwater flow rate through the host rock required by the calculation case definition. Note that, as a general rule, flow rates are specific to each calculation case and thus do not form part of the general modelling approach. In most cases, no-flow conditions are imposed at the lateral boundaries of the model. If the host rock shows a pronounced anisotropy in hydraulic conductivity, this is accounted for in the near-field model.

For calculation cases in which a tectonic-structural element that conducts water in the horizontal direction intersects a cavern, additional, fixed head values are set where this element meets the lateral boundaries of the 3D model (see Section 5.3.1). The determination of all boundary head values is then based on a reference location in the middle of the intersecting geological element.

Nuclide transport in the L/ILW near field model occurs by advection / dispersion and by molecular diffusion, with retardation by linear sorption equilibrium between aqueous phase and solid phases. Heterogeneity, both at the microscopic and the macroscopic level gives rise to mechanical dispersion, which may be anisotropic and is conceptualised as a diffusion-like process with global parameter values (see Section 5.3.6). As described in Section 3.2.6, in modelling the L/ILW near field with VPAC, the selected value of the VPAC input parameter element-specific porosity ε^E for a given nuclide reflects the porosity accessible for advective transport; the pore diffusion coefficient D_p^E (possibly anisotropic) is scaled such that the product $\varepsilon^E \cdot D_{p,\text{scaled}}^E$ yields the effective diffusion coefficient required by the calculation case definition.

Colloid-facilitated nuclide transport is not modelled explicitly (see the discussion in Wieland 2014). The cementitious materials are further assumed to contain only negligible amounts of charged particles; thus the complete pore space is modelled as being accessible to all nuclides. On the other hand, only a fraction of the cement matrix may be assumed to contribute to nuclide retention (see Wieland 2014). At no-flow boundaries, solute transport boundary conditions of type $\partial c/\partial n = 0$ are set. At all other boundaries, $c = 0$ is set (see Fig. 5-3).

ILW

Due to the expected absence of water-conducting, tectonic-structural elements that intersect the emplacement rooms and due to the low hydraulic conductivity of the surrounding undisturbed Opalinus Clay host rock, radionuclide release from the ILW emplacement rooms is expected to be dominated by essentially radial diffusion into the host rock. Nevertheless, in the host rock part of the model, a groundwater flow rate Q is set to also account for advection. This flow rate is calculated as:

$$Q = w_c \cdot L \cdot K_v \cdot i_v \tag{5.3-4}$$

with

w_c	flow capture width of the emplacement room [L]
L	length of the emplacement room [L]
K_v	vertical hydraulic conductivity of host rock [L/T]
i_v	ambient vertical hydraulic gradient across the host rock [L/L]

The flow capture width w_c of the emplacement room is a measure for the amount of groundwater flowing through the host rock that is intercepted by the emplacement room. As illustrated in Fig. 5-4, it is defined as the width of the streamtube that passes through the emplacement room, before it converges on the room. For an elliptical, highly conductive emplacement room in an anisotropic rock, the flow capture width is obtained from potential theory to be:

$$w_c = w + h \cdot \sqrt{\frac{K_h}{K_v}} \qquad (5.3\text{-}5)$$

where width w and height h are the axes of the elliptical room profile normal and parallel to the vertical flow direction, and K_h and K_v are the hydraulic conductivity values of the host rock normal and parallel to the vertical flow (see Nagra 2014c).[68] Since, in the near-field model for ILW, the emplacement room is modelled as a circular, cylindrical feature, w and h take the same value. As discussed in Section 5.3.1, the extent of the EDZ will be small compared to the dimensions of the room and can therefore be neglected when calculating the flow capture width.

Within the ILW emplacement rooms, nuclide concentrations are assumed to be uniform as a result of the high diffusive transport capacity of the backfill material in comparison with the overall solute transport capacity of the host rock. As for L/ILW, the complete pore space of the cementitious materials is expected to be accessible to all nuclides and colloidal nuclide transport is not modelled explicitly.

In the host rock part of the ILW near-field model, nuclide transport occurs predominantly by advection and by molecular diffusion. Mechanical dispersion is expected to be a minor process, given the very low rates of advection in the Opalinus Clay host rock. Because transport in the host rock part of the near-field model is represented as a 1D process, anisotropic diffusion is not explicitly accounted for. Rather, effective diffusion coefficients for transport parallel to bedding, which are higher than those normal to the bedding, are pessimistically applied. Nuclide transport in the host rock part is retarded by linear equilibrium sorption; precipitation / redissolution of nuclides is not modelled.

A $c = 0$ condition is set at the outer boundary of the host rock part of the near-field model (see Fig. 5-4).

SF / HLW

As described in Section 5.3.1, solute transport in the SF/HLW emplacement rooms is expected to be dominated by radial diffusion. As for ILW, a groundwater flow rate Q is set in the host rock part of the near-model to also account for advection. This flow rate is calculated using eq. 5.3-4, with the difference that L denotes the length of a SF or HLW canister plus the distance between two adjacent canisters. Unlike the case of ILW, an SF/HLW emplacement room is not overall a highly conductive feature, since it is backfilled with a compacted bentonite buffer. Nevertheless, the capture width w_c may still be calculated with eq. 5.3-5, based on the assumption that the room has a cementitious liner with a higher hydraulic conductivity than the host rock. As in the case of ILW, the EDZ is not taken into account in calculating the flow capture width.

[68] This formula is applicable when it is assumed that the seals at the end of the emplacement rooms are tight, such that water flow along the emplacement room does not occur.

Dissolved nuclides diffuse from the reservoir (i.e. the canister interior) into the buffer, but those associated with solids, including e.g. precipitated colloids, are retained within the reservoir since the buffer provides an effective filter for such materials. Sorption on solid surfaces inside the canister (including the internal surface of the metal canister itself and its corrosion products) is not taken into account.

In the bentonite buffer, diffusive transport of some nuclides is retarded by linear, equilibrium sorption between the aqueous phase and solid phases. Solubility limits constrain nuclide concentrations in the buffer, as in the canister interior. Only the concentrations of isotopes originating from the waste forms are taken into account in evaluating whether solubility limits are exceeded. The background concentrations of stable isotopes originating from other materials are conservatively ignored. In contrast to the cementitious materials in the L/ILW and ILW near-field models, element-specific porosity values are specified for the bentonite buffer, e.g. to account for anion exclusion.

With respect to nuclide transport in the host rock part of the SF / HLW near-field models, the same assumptions as for ILW apply (see also Fig. 5-5).

5.3.4 Long-term evolution

The effective containment zones in the geological siting regions are characterised by very low permeability. A specific calculation case may, however, be defined to investigate the influence of decompaction of the effective containment zones on their permeability and hence on radionuclide release from the barrier system. In this case, a time-dependent water flow rate in the host rock is specified in the near-field models, consistent with the prescribed flow rate in the geosphere models (see Section 5.4.4).[69]

Other potential long-term effects in the near field (e.g. volume change due to corrosion of steel) are considered to be of low relevance to the nuclide release rates (Bradbury et al. 2014, Kosakowski et al. 2014) and are therefore not modelled explicitly.

5.3.5 Interface with the geosphere

For all types of near-field model, radionuclide release from the near field is evaluated at a 1 m distance from the external boundaries of the emplacement rooms inside the undisturbed host rock. The use of this location as the interface with the geosphere, rather than the outer boundaries of the emplacement rooms themselves, is motivated as follows:

- Because of the way in which the near-field and geosphere computer codes are coupled, with releases calculated by the near-field code providing the source term for the geosphere code, any nuclide fluxes that take place in the reverse direction (i.e. from the geosphere model domain to that of the near field) cannot be modelled. Such reverse fluxes may, however, occur in reality at the outer boundaries of the emplacement rooms. Note that nuclide fluxes across these boundaries are always significantly influenced by the surrounding geosphere, due to differences in transport and retention properties between engineered materials and the geological environment. This is particularly the case for the cementitious near field of the ILW and L/ILW emplacement rooms, in which, for example, chemical conditions are significantly different compared with the different host rocks. This contrast may – under certain circumstances – lead to reversed fluxes of daughter nuclides back into the emplacement rooms (see Nagra 2009).

[69] Additional time-dependent water flow and solute transport calculations are documented in Kosakowski (2004), although the effects investigated there are beyond the scope of the present dose calculations.

- Experience from earlier safety assessments shows that evaluating nuclide release at 1 m inside the host rock substantially reduces the number of nuclides released to the geosphere, given the excellent sorption properties of all candidate host rocks (more specifically: the host rock in its strict sense). The near-field results are thus easier to understand and to compare between different siting regions. Another benefit is that geosphere modelling may be computationally more efficient if fewer radionuclides are considered. Note that 1 m is a rather small value compared with the overall vertical extent of all candidate host rocks and with the assumed spacing between emplacement rooms.

5.3.6 Code selection and numerical aspects

L/ILW

Because modelling of the L/ILW near field needs to be carried out in three dimensions for certain calculations cases (see Section 5.3.1), the code VPAC 1.1 is used for all L/ILW near-field calculations. A detailed description of the code, including the underlying assumptions, the input requirements, the solution method and the principal verification steps, is given in Section 3.3.

VPAC 1.1 requires a 3D finite-element mesh (FE mesh) for calculating near-field releases from L/ILW emplacement caverns. Fig. 5-6 shows the standard FE mesh for an emplacement cavern of type K09, which is derived from the geometrical specifications in Fig. 5-3. For symmetry reasons, only half of the cavern (with respect to the cavern width) is modelled. The standard mesh consists of 5'685 irregular finite elements and the width of the single layer in the third dimension is 1 m (quasi-2D mesh). For a smaller emplacement cavern of type K04, a similar mesh with the same number of elements is used. All materials treated separately in the model are represented as homogeneous porous media.

Fig. 5-7 shows a variant FE mesh, which accounts for a single vertical fault intersecting a L/ILW emplacement cavern of type K09, with vertical flow within the fault. The cavern has an overall standard length of 200 m. However, since the fault is assumed to intersect the cavern mid-way along its length, the symmetry of the system can be exploited and only half of the cavern needs to be modelled. This mesh comprises 79'590 irregular finite elements (14 layers of 5'685 elements, meaning that each layer contains the same number of elements as the standard FE mesh shown in Fig. 5-6). An alternative mesh for a single vertical fault intersecting a L/ILW emplacement cavern of type K04 also consists of 79'590 elements. In both cases, the fault is modelled explicitly as a homogeneous porous medium with a width of 10 cm. However, because of the above-mentioned use of symmetry, only half of the fault width (5 cm) is included in the mesh.

The hydraulic conductivity of the fault is set according to the transmissivity specified in the calculation case definition. The total porosity is set to 1 %, which, together with the assumed width of the fault, is equivalent to an open flow channel with a thickness of 1 mm and porosity of unity for all nuclides, as used in the corresponding geosphere modelling approach described in Section 5.4.3. The sorption coefficients for all nuclides are conservatively set to zero and the element-specific pore diffusion coefficients for diffusion in free water are applied (values taken from van Loon 2012).

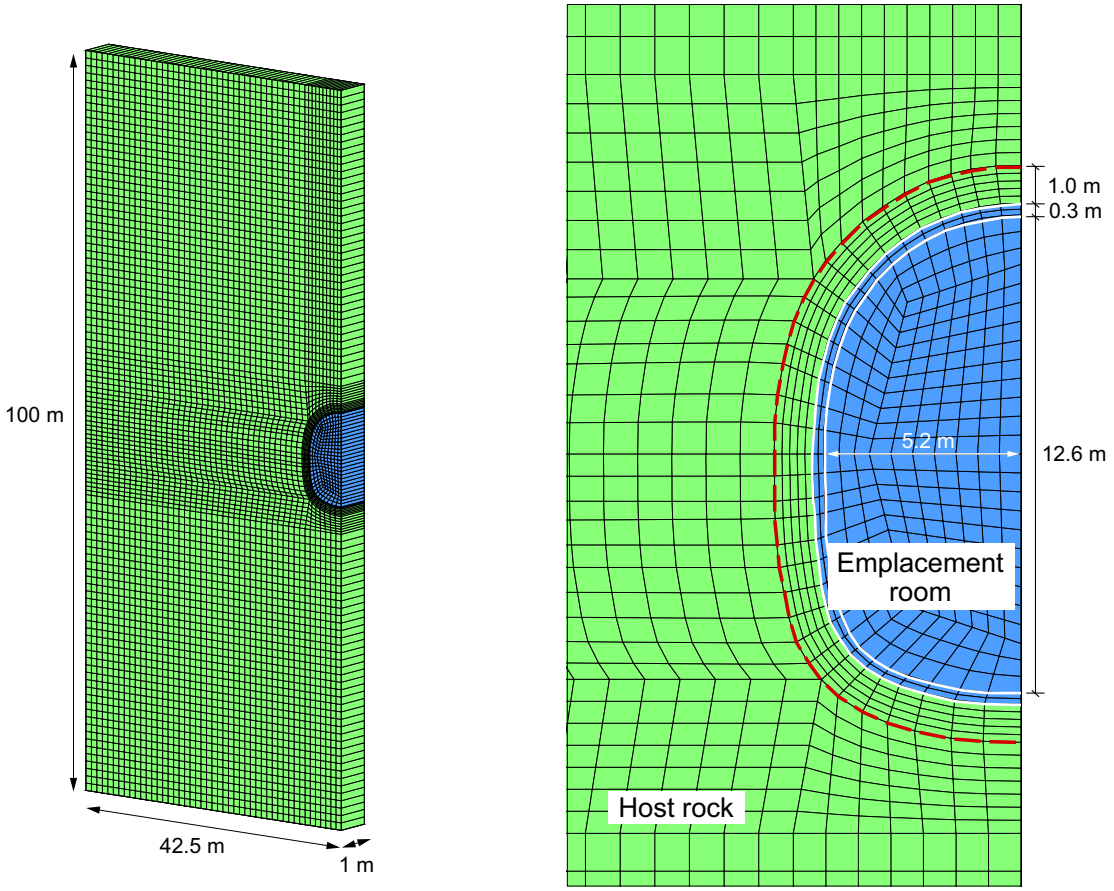

Fig. 5-6: Standard FE mesh used to calculate near-field release from L/ILW emplacement caverns of type K09.

Fig. 5-8 shows a variant FE mesh for the smaller cavern type K04, which also accounts for vertical faults with a typical spacing of 100 m intersecting with the emplacement cavern, but for a situation in which flow in the fault is on average in the horizontal direction and restricted to a rock unit of 5 m thickness that intersects with the cavern. This mesh comprises 71'932 irregular finite elements. All other modelling assumptions are the same as for the situation with vertical flow orientation within a vertical fault.

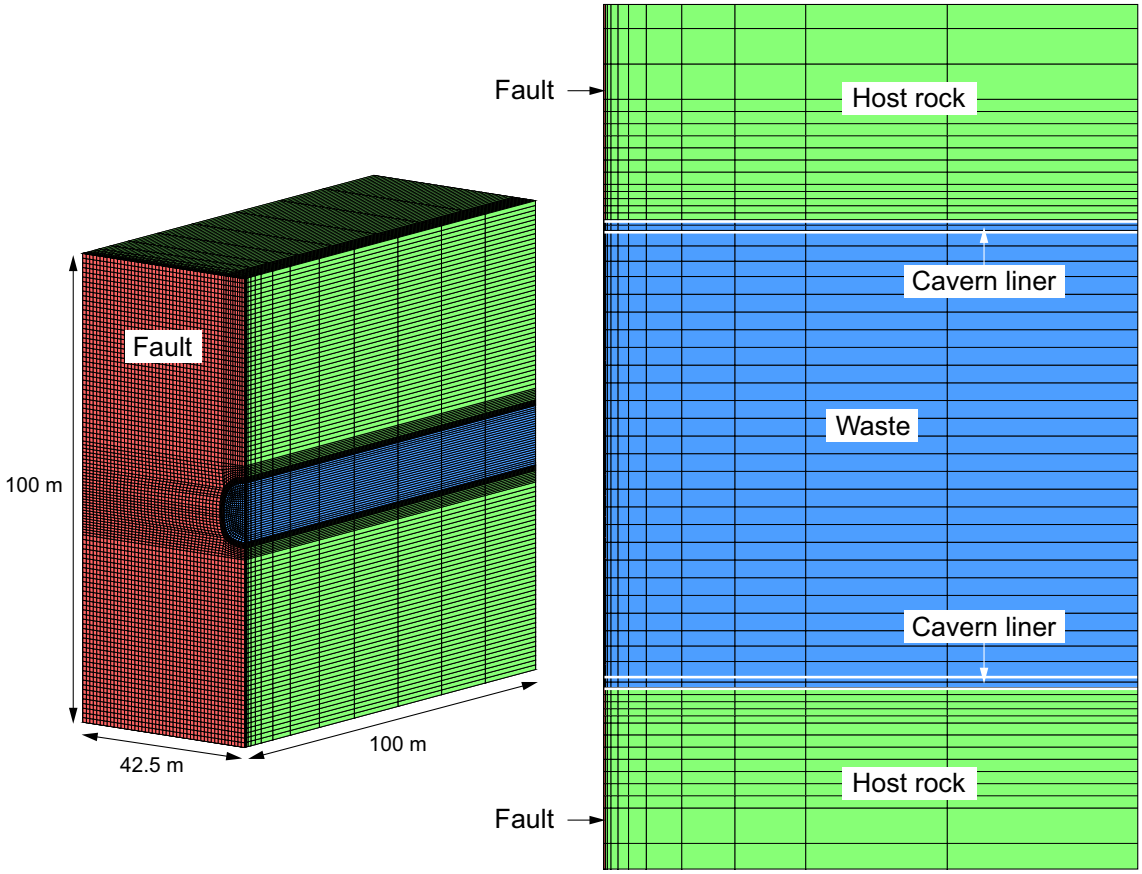

Fig. 5-7: FE mesh used to calculate near-field release from a L/ILW emplacment cavern of type K09 for vertical faults with a typical spacing of 100 m and with vertical flow orientation within the fault.

If the calculation case definition requires the host rock to be conceptualised as a medium with densely-spaced water-conducting features (e.g. joints), these features are not modelled explicitly, but rather by means of equivalent water flow and solute transport parameters. These equivalent parameters are derived from the case-specific parameters of the rock matrix and from those generally assumed for discrete water-conducting features, as described above (see also Section 5.4.3), based on the following assumptions:

- the large-scale hydraulic conductivity of the rock (including anisotropy if any) is respected,
- the total pore volume of the rock is respected, i.e. an average pore volume is calculated,
- the total mass of the rock is respected, i.e. an average bulk dry density is calculated,

- The transport paths through the matrix and the transport path through the discrete water-conducting features are calculated separately,
- the initial dispersive / diffusive flux into the host rock is respected.

Test calculations have shown that this approach may not be conservative in all cases. However, the differences in the calculated total dose rate compared with that calculated using a 3D modelling approach are very small.

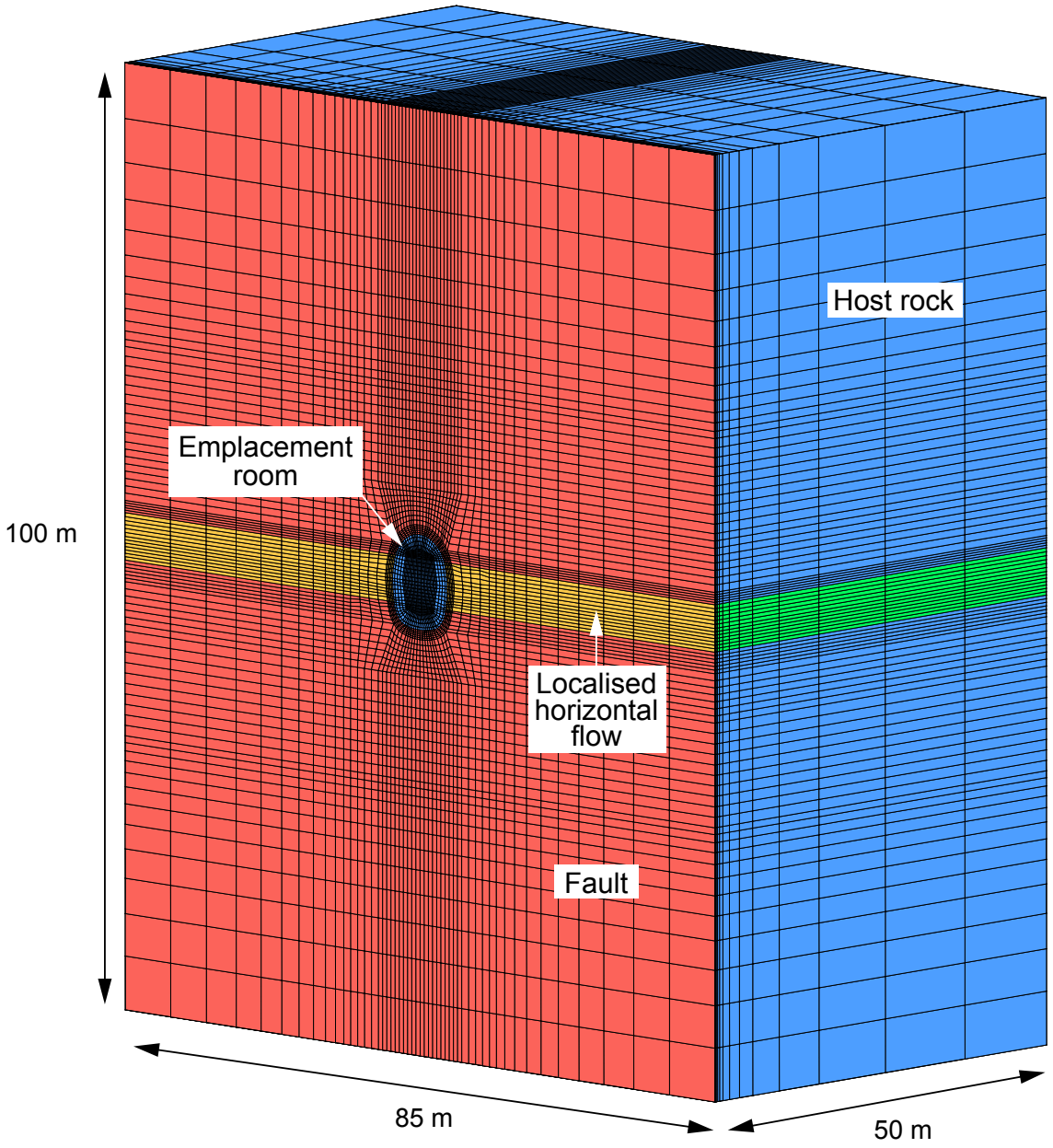

Fig. 5-8: FE mesh used to calculate near-field release from a L/ILW emplacment cavern of type K04 for vertical faults (red colour) with a typical spacing of 100 m intersecting the emplacement cavern and with localised horizontal flow within the fault (orange colour).

To ensure that the time and space discretisations used in VPAC calculations produce an accurate solution, the time step size must respect the Neumann criterion (Charney et al. 1950):

$$Neu = \frac{2 \cdot D \cdot \Delta t}{h_d^2} \leq 1 \qquad (5.3\text{-}6)$$

where D is the hydrodynamic dispersion coefficient, h_d is the element size and Δt is the time step. Longitudinal and transverse dispersion coefficients of 2 m and 0.2 m[70], respectively, are used throughout the modelled near-field domain,

The computation time for a VPAC calculation depends on the calculation at hand. It varies from a few minutes to more than one day for the variant mesh with horizontal flow along a fault. In the latter case, several calculations are run in parallel for different groups of nuclides to circumvent computer memory constraints.

ILW and SF / HLW

The STMAN 5.9 suite of codes is used to calculated ILW and SF/HLW near-field release and transport, because the near field in these cases is adequately described using cylindrical geometry (no water-conveying faults in the Opalinus Clay host rock are expected). This choice of codes is further motivated by the fact that, for ILW and SF / HLW near-field modelling, solubility limitation is explicitly taken into account, in which case STMAN is far more efficient than VAC from a computational standpoint. A detailed description of STMAN, including the underlying assumptions, the input requirements, the solution method and the principal verification steps, is given in Section 3.4.

With STMAN, the model domain is discretised into a number of finite-difference (FD) cells of various types. The cell types include waste cells, reservoir cells, buffer cells, host rock cells and mixing cells. The buffer, host rock and mixing cells are the same for all near-field models, while the waste cells and reservoir cells are specific to the type of near field being modelled.

The number of cells used to discretise the buffer is set by the user. Typically, a few tens of cells are sufficient. When the diffusive host rock layer option is used, the number of cells for the host rock is also set by the user and the cells can be made progressively larger as distance from the buffer increases. Note that the discretisation of the host rock is adjusted internally by the code, so that the position where the near-field release is reported lies exactly on a cell boundary.

The computing time of an STMAN calculation is typically in the order of minutes.

5.4 Geosphere

In this section, the generic aspects of modelling transport of dissolved radionuclides in the geosphere are explained in detail. The description is rather broad, since a variety of water flow and solute transport situations may need to be investigated in the dose calculations. A number of assumptions may appear rather stylised, which is due the fact that, at the current stage of repository implementation, information about the exact location of individual waste packages, emplacement rooms and tectonic-structural elements in the geological environment and their orientation relative to each other is yet not available.

[70] The choice of these parameter values is motivated by the extent of L/ILW emplacement rooms and also takes account of the effects of numerical dispersion. It turns out that the calculated near-field release rates are rather insensitive to these parameter values.

5.4.1 Description of domain

The geosphere domain of a given emplacement area is modelled as a vertical stack of rock units, as illustrated in Fig. 5-9. Because the near-field domain containing the emplacement rooms is modelled separately from the geosphere domain, the latter actually consists of two vertical stacks of rock units: one stack above and the other below repository level.

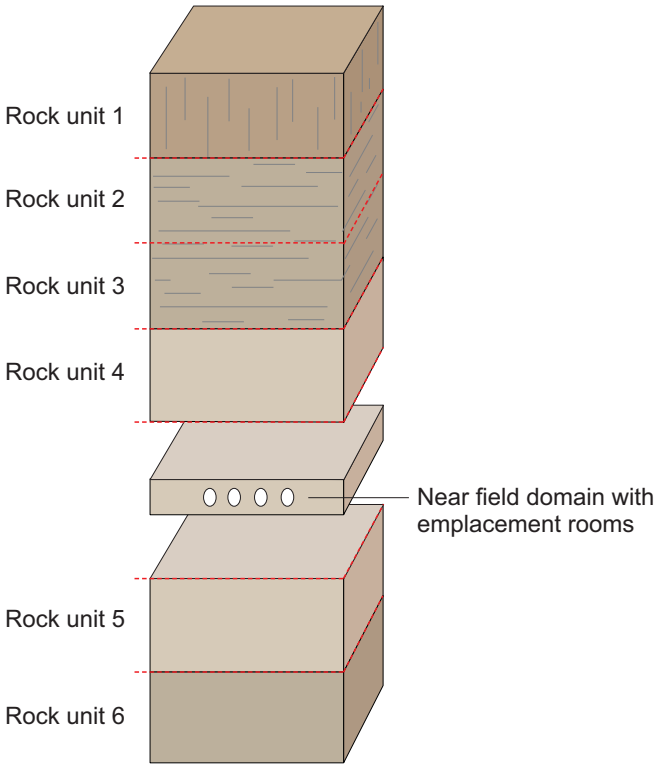

Fig. 5-9: Illustration of the geosphere model domain consisting of different rock units.

In the present context, rock units are classified in a manner that is appropriate to radionuclide transport modelling,[71] since each rock unit differs from those adjacent to it in its (large-scale) water flow and solute transport properties. The specification of the properties defining each rock unit is closely linked to the definition of the individual calculation cases and is thus within the scope of Nagra (2014b). For all rock units, saturated hydraulic conditions are assumed.

The individual rock units are assumed to have horizontal upper and lower boundaries. In other words, they have a uniform thickness across the complete emplacement area under consideration. Fig. 5-10 shows some examples of rock units and fault settings considered in geosphere modelling in the context of the present dose calculations.

[71] It is thus different from other types of rock classifications, such as classifications based on stratigraphy or current hydrogeological conditions.

Most rock units are conceptualised as homogeneous porous media (HPM), possibly with anisotropic water flow and solute transport properties, which means that all heterogeneity on a macroscopic scale is averaged over the entire rock unit (see pictures a) and b) in Fig. 5-10). For instance, the physical quantities porosity and hydraulic conductivity of the host rock, which are used as input parameters to the geosphere model, represent average values for the whole host rock unit.

Fractured rock units, i.e. rock units with discrete discontinuous features, are conceptualised in the geosphere model as a homogeneous and possibly anisotropic porous rock matrix that is interspersed with regularly spaced, vertical, planar flow features (see picture c) in Fig. 5-10). Flow along such features may be horizontal or vertical, depending on the site-specific concept of radionuclide transport for the calculation case at hand. Radionuclide exchange between these flow features and the matrix occurs via diffusion perpendicular to the surfaces of the features. The mathematical model applied to such situations is described in Section 3.2.7. Note that, in this report, the terms fracture, discrete (water-conducting) flow feature and transmissive element are used as synonyms and that they can refer to phenomenologically different tectonic-structural elements, such as faults, joints, fissures and slip surfaces.

The entire ECZ may be interspersed with large-scale tectonic-structural elements, termed faults. With respect to such faults, it is assumed that these

- extend vertically and horizontally throughout the entire ECZ of an emplacement area, i.e. through all rock units present in the ECZ,
- have water flow and solute transport properties that can vary between the rock units that they intersect, and
- meet the emplacement rooms at right angles to the room axes, thus affecting all emplacement rooms equally.

The pictures d) and e) in Fig. 5-10 illustrate these assumptions. In picture d), the ECZ is affected by a single fault with enhanced transmissivity in all rock units, thus resulting in vertical flow within the fault, in addition to the ambient vertical flow in the adjoining rock matrix. In picture e), the ECZ is affected by several faults, which in most rock units do not show a significantly higher hydraulic conductivity compared with the undisturbed part of these rock units. In one rock unit, however, they do have a significantly higher hydraulic conductivity, thus potentially allowing for horizontal water flow and solute transport along this rock unit (see Nagra 2014b for the definition of such calculation cases). If one or more faults with elevated hydraulic conductivity intersect the emplacement rooms, then specific near-field models for L/ILW are used (see Section 5.3.6).

All fractures are modelled as thin open channels with an aperture of 1 mm.[72] Following the notation in Section 3.2.7, this means that $2b = 1$ mm (see also Fig. 5-10). The assumed regular spacing of the fractures takes the value $2B$. Thus, the extent of the accessible rock matrix is $(B - b)$ on both sides.[73] If a single fault is considered, it is assumed to cut the emplacement rooms at their mid points and – because the lateral boundaries of the ECZ are considered impervious – the lateral extent of the rock matrix on either side of the centre of the fault (B) is limited to half of the length of the emplacement rooms L ($2B = L$, see also Section 5.3.6).

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[72] This choice is motivated by the fact that the PICNIC-TD input parameters (i) infill porosity and (ii) fracture aperture are correlated, and that radionuclide transport is relatively insensitive to both of these parameters.

[73] Note that, using the geosphere code PICNIC-TD, several identical transport paths can be modelled with a single leg (see Section 3.5.5). This approach is taken, e.g. to model a regular pattern of small-scale tectonic-structural elements (joints).

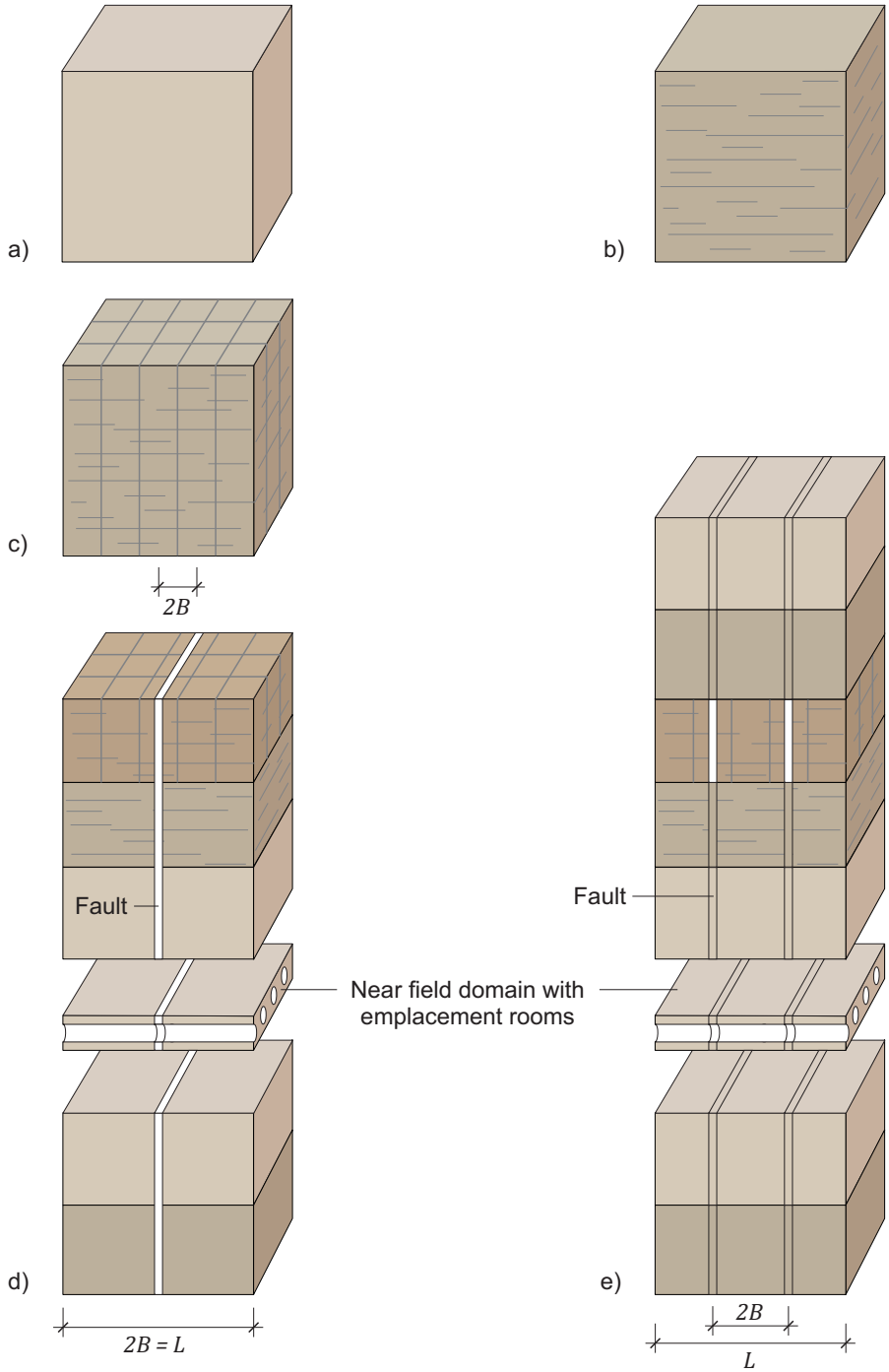

Fig. 5-10: Examples of rock units and fault settings considered in geosphere modelling.
a) homogeneous porous medium (HPM), b) HPM with anisotropy, c) jointed medium with anisotropy in matrix, d) effective containment zone (ECZ) affected by a single fault (vertical flow in the fault), e) ECZ affected by several faults with variable transmissivity in different rock units (potentially horizontal flow in individual fault sections, white areas).

In some calculation cases, the rock matrix between faults may need to be modelled as a jointed medium. In such cases, two parallel transport paths are modelled: one for the faults and the adjoining rock matrix, and one for the remaining jointed rock volume not affected by the faults (see picture e) of Fig. 5-11)[74].

If the geosphere comprises an alternating sequence of rock units with just two different sets of transport properties, the sequence is, for simplicity, reordered to group together the units with the same properties, such that it, in effect, comprises two grouped rock units. The type of reordering that yields the highest total maximum dose rate is, in general, specific to the calculation case at hand, which – from a modelling point of view – is rather inconvenient, since a number of variants may need to be analysed for each calculation case. On the other hand, preparatory analyses for relevant types of rock units have shown that the differences in total maximum dose rate are small for these variants (see Hayek et al. 2014). Therefore, no requirement has been established with regard to the way the reordering is carried out.

5.4.2 Source term

The source term for each geosphere model is built from the sum of radionuclide release rates from the individual near-field models for the emplacement area under study.

If the host rock shows small-scale discontinuous features (e.g. due to the presence of joints), then the entire radionuclide release from the near-field model, in which such host rock is conceptualised as an equivalent porous medium (see Section 5.3.1), is conservatively fed into the discrete flow features (host rock legs, see below) in the geosphere model.

In case of large-scale faults intersecting with the L/ILW emplacement caverns, the results from the near-field model described in Section 5.3.6 are post-processed to obtain separately the releases to these large-scale geological features and the releases to the rock matrix. The relevant fractions of the near-field release are then assigned to the corresponding features in the geosphere model.[75]

In all cases, the source term is applied at the junction between the legs representing the stack of rock units above the repository level and the legs representing the stack below the repository level (see Fig. 5-11).

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[74] The extent of the matrix of the fault is in this case limited to half the spacing of the joints.

[75] For instance, if the host rock consists of a homogeneous porous medium intersected by faults, radionuclide release to the faults calculated by the near-field model provides the source term for the representation of the faults in the geosphere model and the remainder is taken as source term for the undisturbed host rock in the geosphere model.

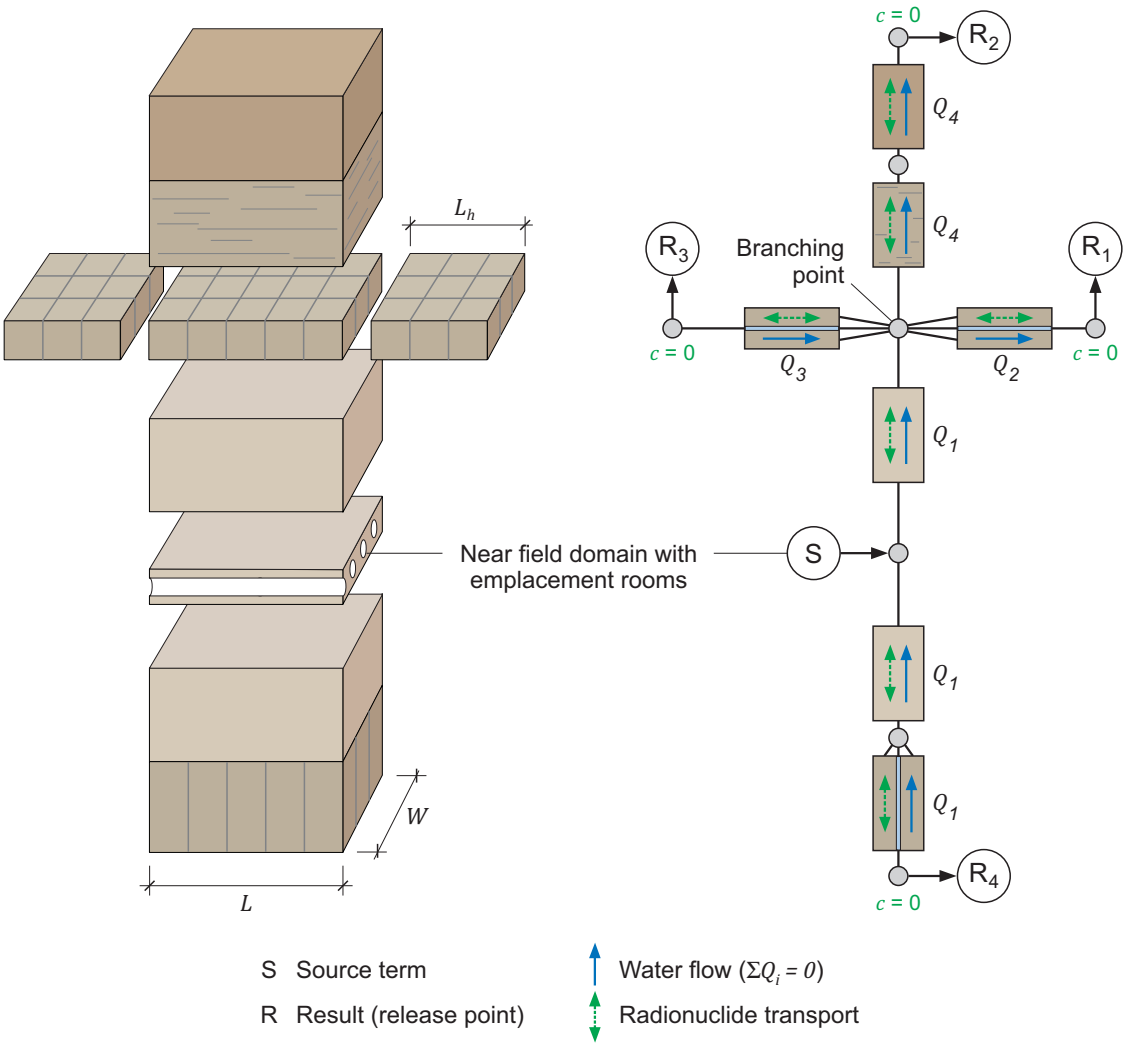

Fig. 5-11: Example of the conceptualisation of water flow and radionuclide transport as a network of one-dimensional flow and transport pathways (legs).

5.4.3 Water flow and solute transport

Water flow and solute transport in the geosphere is modelled in a network of one-dimensional pathways, called legs. In most cases, each leg corresponds to an individual rock unit and, for vertical legs, the leg length is equivalent to the thickness of the rock unit under consideration. An example of a network of legs is given in Fig. 5-11.

In the geosphere model, water flow is not calculated, but rather it is prescribed individually for each leg. As a general rule, total water flow is always determined by the specifications of the calculation case to be analysed, and thus does not form part of the general modelling approach. Note that, for the determination of water flow, the vertical hydraulic gradient along any fault is assumed to be the same as that across the adjacent rock matrix, regardless of the assumed fault transmissivity.[76]

[76] In reality, the gradient along, and in the immediate vicinity of, the fault is expected to be reduced compared with the gradient across the more distant parts of the rock matrix. The adopted approach is thus pessimistic.

When using the transport code PICNIC-TD, it is of vital importance that water flow in the geosphere model domain be prescribed in a consistent manner (see also Section 5.4.5). Since there are no sources or sinks of water within the model domain, all water fluxes at leg junctions must sum to zero. It also implies that all water fluxes across the boundary of the geosphere model domain also sum up to zero, as indicated in Fig. 5-11.

Radionuclides released from the near-field model are transported away from the repository level by advection and by molecular diffusion along the legs. Furthermore, heterogeneity at both the microscopic and the macroscopic levels gives rise to mechanical dispersion in flow direction. Transverse dispersion is not modelled, in line with the one-dimensional modelling approach in the geosphere. Transport of radionuclides may be retarded by linear, equilibrium sorption. As noted earlier, only trace amounts of radionuclides are expected to reach the geosphere. Hence, no constraints on nuclide solubility are set and stable nuclides need not be considered in the geosphere model. As illustrated in Fig. 5-11, a transport boundary condition of type $c = 0$ is conservatively set at all release points from the leg network.

If a leg represents a discrete transmissive element (e.g. fault or joint) and its rock matrix, diffusive transfer between the transmissive element and the matrix is additionally taken into account. The transmissive element itself is modelled as an open channel of porosity $\varepsilon = 1$ and the retardation coefficients of all nuclides migrating within the channel are conservatively set to unity ($R^E = 1$). Further, the element-specific pore diffusion coefficients for diffusion in free water are applied (van Loon 2012).

Radionuclide transport in the matrix adjacent to a discrete flow feature occurs by diffusion. Matrix diffusion is modelled as a 2D process in a vertical plane normal to the surfaces of the flow feature and may be anisotropic. In case of a fault with vertical water flow, advection and dispersion parallel to flow direction in the fault are additionally taken into account. In calculation cases that investigate the potential effects of colloid-facilitated transport in fractures, the colloids are assumed to be prevented from entering the rock matrix due e.g. to their size or charge (see Nagra 2014b).

With regard to the type of connection between geosphere legs, there are several possibilities (see Fig. 5-12):

a) The most frequent case is the situation in which a homogeneous porous medium is in contact with another homogeneous porous medium.

b) Where there is a discrete transmissive element that extends over both rock units (e.g. a fault), then there is a link between the parts of the element that are in each of the units, and a separate link between the remaining parts.

c) If one rock unit represents a HPM and the other rock unit has a discrete transmissive element, then the HPM is connected to both the transmissive element and the adjoining matrix of the other rock unit. This implies that mixing conditions are assumed between the two rock units.

d) Similarly, if both rock units contain discrete transmissive elements, but these are of different kinds (e.g. of different spacing), then the radionuclide flux is routed through a single junction, which means that mixing conditions between the two rock units are assumed, as in c).

e) If each rock unit is represented by two separate legs, each leg of one unit is linked to the corresponding leg of the other unit according to the rules a) to d).

If more than two transport paths are linked together, then mixing conditions are generally assumed, regardless of the types of transport path in the individual rock units.

Modelling horizontal transport along a tectonic-structural element (as in the example in Fig. 5-11) is a particular case where mixing conditions are applied at leg junctions. The tectonic-structural element and its associated matrix are assumed to extend to a distance L_h beyond the lateral boundaries of the ECZ. Note that horizontal transport is only modelled outside the lateral boundaries of the emplacement area, since within the ECZ only 1D transport in the vertical direction is accounted for (see Section 5.4.1). All along the horizontal transport path outside the lateral boundaries of the emplacement area, diffusive exchange with overlying and underlying rock units above is, for simplicity, not considered. This is pessimistic with regard to radionuclide transport along the horizontal path. Note further that there are always two horizontal legs present (as illustrated in Fig. 4.5-3), in order to provide for consistent water fluxes at the branching point. If the horizontal legs model a discrete flow element, no water flow is assumed in the matrix adjacent to this element (see above).

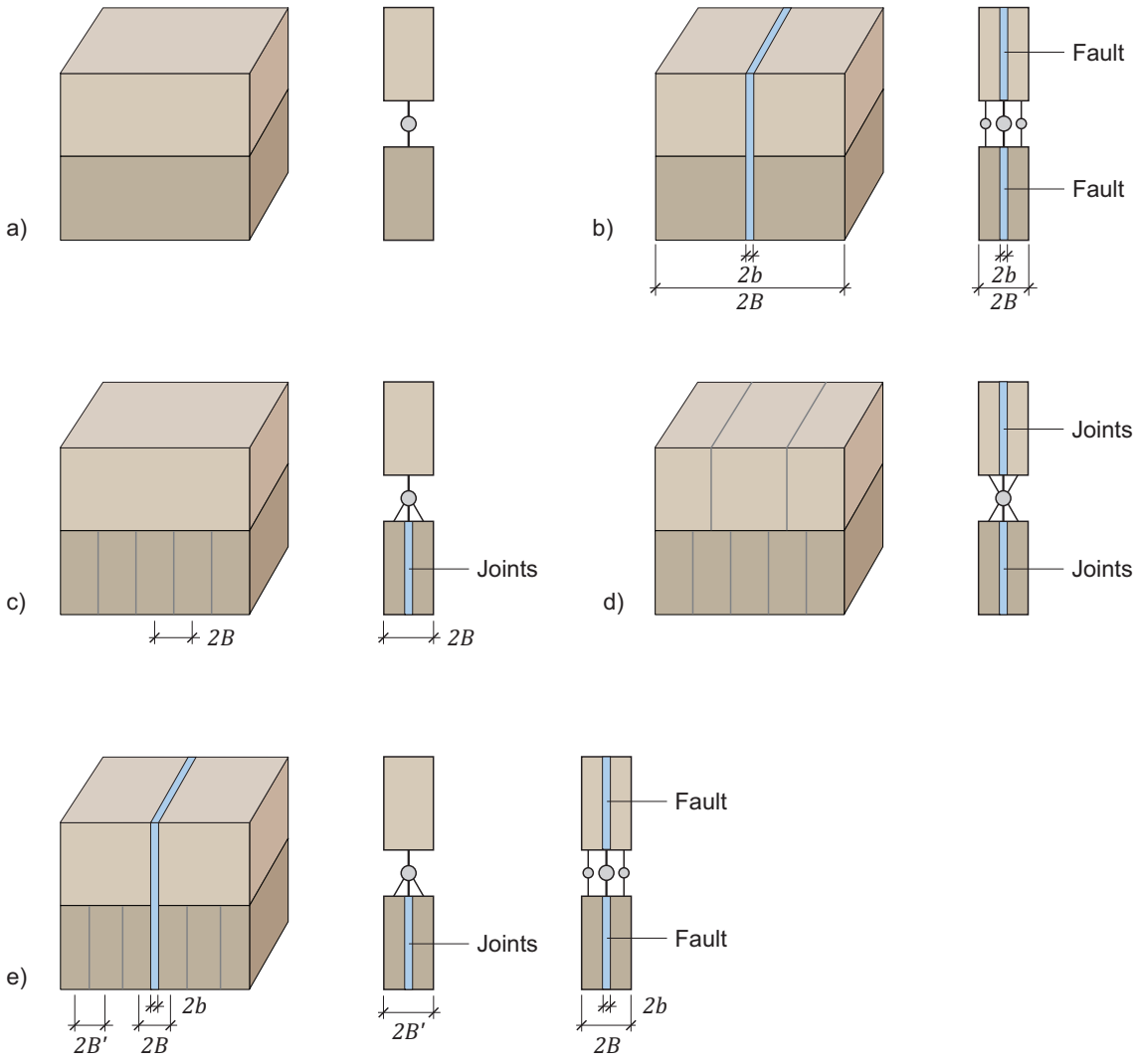

Fig. 5-12: Conceptualisation of rock units with different leg types, including possible types of connection between legs.

With respect to the direction of horizontal water flow and radionuclide transport, it is usually assumed that these occur parallel to the emplacement rooms, as in Fig. 5-11. This assumption maximises the contact area of the horizontal paths with the ECZ, thus also maximising their total transport capacity, all other parameters being equal.[77] However, if horizontal transport occurs along one or several faults (regardless of whether horizontal transport in the faults is at repository level or not), the horizontal transport orientation is assumed perpendicular to the emplacement rooms, since faults are in the L/ILW near-field models assumed to intersect with the emplacement rooms at right angles (see Section 5.4.1).

5.4.4 Long-term evolution

As noted in Sections 5.2 and 5.3.4, a specific calculation case may investigate the influence of decompaction of the ECZ on water flow and solute transport properties and hence on radionuclide release from the barrier system. In this case, it is assumed that the rate of change of groundwater velocity is small, and thus the same rate of change throughout the model domain is assumed.

5.4.5 Code selection and numerical aspects

Because radionuclide transport in the geosphere is principally conceptualised as a one-dimensional transport phenomenon, the code PICNIC-TD 1.4 is applied. A detailed description of the code, including the underlying assumptions, the input requirements, the solution method and the principal verification steps, is given in Section 3.5.

A fundamental difference between PICNIC-TD and its predecessor PICNIC, which was the standard code for geosphere modelling in earlier safety assessments of Nagra, is the use of a spatial discretisation for the solution of the transport equation in PICNIC-TD. This has two principal advantages:

- it allows the consideration of transient water flow in solute transport modelling, and
- the partitioning of radionuclide fluxes at junctions between two or more legs is treated more realistically in that the advective / dispersive and diffusive transport capacities of the connected legs – and hence the splitting of radionuclide fluxes – are evaluated automatically and dynamically by the code (concept of a shared concentration).

Note that two preconditions for the validity of the approach adopted in PICNIC-TD are the consistent specification of (i) the cross-sectional areas of legs meeting at a junction and of (ii) the total water flow within these legs (see Sections 3.5 and 5.4.3).

In contrast to PICNIC, where two parallel legs are needed to model advective / dispersive transport in a discrete transmissive element (also termed fracture) together with advective / dispersive transport in the associated matrix, a single leg suffices to represent such a system in PICNIC-TD (see Section 5.4.3). If not specified explicitly, the discrete flow channel of the transmissive element is discretised in flow direction into a number of cells of constant length. The number of cells, m, depends on the Peclet number Pe and two user-defined parameters, n and v: $m = n + v \cdot Pe$. The matrix is discretised in flow direction using a uniform grid, which matches the flow channel discretisation. A Peclet number of $Pe = 10$ is used for all geosphere calculations. Previous tests have shown that the calculated maximum dose rate is not sensitive to this parameter value.

[77] For all emplacement areas, the total width W is greater than the length L (see Nagra 2014b).

In the direction perpendicular to flow, the matrix is discretised using a method that combines a compartment discretisation scheme with a Taylor Series discretisation scheme. The matrix is divided into a number of layers, the default number of layers being 10. Starting at the layer interfacing with the fracture, the thickness of the layers increases progressively by a factor of 2.5 (default) from one layer to the next. If the extent of the accessible rock matrix is in the order of meters or less, the default number of layers is sufficient to obtain accurate results. However, for a larger accessible matrix (e.g. 100 m, as in the situation of a single fault within a homogeneous porous medium intersecting with an L/ILW emplacement room), the first layer (close to the fault or fracture) has a thickness of around 0.055 m if the default discretisation schemes is used, which numerical tests have shown to be too large to give accurate results due to an underestimation of the nuclide exchange between fracture and matrix. Increasing the number of layers improves accuracy, but also increases computation time. As a compromise, a sub-division into 17 layers has been found to be an optimum solution for an extent of accessible rock matrix in the order of several hundreds of meters. With this approach, the first layer has a thickness of about 10^{-4} m, which is similar to that obtained for a 0.5 m accessible rock matrix using the standard subdivision into 10 layers. More details on the approach to modelling solute transport within a fracture are given in Section 5.4.3.

Using the default values for the solver accuracy parameters that control time-stepping, the computing time for a PICNIC-TD calculation varies from a few minutes to one day.

6 References

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A Relevant Processes and Parameters

Tab. A-1 lists the processes and parameters that are of relevance to the post-closure safety of a deep geological repository from the perspective of the on-going site-selection process (see Nagra 2014b). This table also indicates how each process or parameter is treated in the dose calculations.

As described in Nagra (2014b), the relevant processes and parameters have been identified by Nagra based on:

- the post-closure safety functions and general design principles for a deep geological repository,
- the barrier concepts envisaged (see Fig. 1-1),
- the safety-relevant properties of the elements of the barrier systems,
- regulatory requirements, and
- experience with earlier safety assessments in Switzerland and abroad.

In deriving the list of processes and parameters, the focus has been on site-specific geological aspects, as these are of major importance for the provisional safety analyses and for the safety-related comparison required for SGT Stage 2. Special attention has been given to those aspects of the post-closure safety performance of the engineered barriers that have to be addressed explicitly in the provisional safety analyses following specific requirements set forth in the regulatory guiding document (ENSI 2010b).

Tab. A-1: List of relevant processes and parameters.

In the dose calculations the relevant processes and parameters are either directly accounted for in the models and computer codes (+) or considered implicitly in derived input parameters or via conceptual assumptions based on system analyses (*).

Code	Process or parameter	Treatment in the dose calculations
Processes and parameters related to the engineered barriers		
PT-1	Container lifetime SF / HLW	+
PT-2	Dissolution rate of SF matrix and SF cladding tubes	+
PT-3	Near-field solubility limits for SF / HLW / ILW	+
PT-4	Near-field sorption coefficients	+
PT-5	Advection and diffusion in the near field	+
PT-6	Transport-relevant properties at the SF / HLW disposal tunnel / host rock interface	*
PT-7	Design of waste emplacement rooms	*
Processes and parameters related to the geological barriers		
PG-1	Depth below ground surface with respect to repository exposure by erosion	*
PG-2	Glacially over-deepened valleys	*
PG-3	Depth below ground surface with respect to rock decompaction	*
PG-4	Evolution with time of regional base level of erosion	*
PG-5	Thickness	*
PG-6	Large-scale hydraulic conductivity	+
PG-7	Influence of decompaction on hydraulic conductivity	+
PG-8	Hydraulic gradient	+
PG-9	Type of transport pathways	+
PG-10	Porosity	+
PG-11	Structural-tectonic elements in sedimentary layers	+
PG-12	Location and composition of karstic rocks within the host rock	*
PG-13	Length of transport pathways	+
PG-14	Fault zone transmissivity	+
PG-15	Mineralogy	*
PG-16	pH value	*
PG-17	Redox conditions	*
PG-18	Salinity	*
PG-19	Microbial processes	*
PG-20	Colloid filtration in the geosphere	+
PG-21	Sorption coefficients for host rock / effective containment zone	+
PG-22	Diffusion coefficients for host rock / effective containment zone	+
PG-23	Excavation damage / disturbed zone in the vicinity of underground structures	*
PG-24	Effects of a high-pH (hyper-alkaline) plume on the host rock	+

Tab. A-1: (continued)

Code	Process or parameter	Treatment in the dose calculations
Processes and parameters related to the geological barriers		
PG-25	Host rock behaviour with respect to gas	*
PG-26	Host rock behaviour with respect to temperature	*
PG-27	Relevant groundwater discharge pathways	*
PG-28	Evolution with time of local topography in terms of long-term geological evolution	*
PG-29	Evolution with time of local topography in terms of biosphere modelling	*
PG-30	Climate evolution in relation to long-term geological evolution	*
PG-31	Climate evolution in relation to estimating water fluxes for biosphere modelling	+
PG-32	Conflicts of use with natural resources beneath the host rock	not treated
PG-33	Conflicts of use with natural resources above the host rock	not treated
PG-34	Conflicts of use with geothermal energy resources	not treated

B Management of Calculations

The dose calculations undertaken in the context of the provisional safety analyses need to be managed in a well-defined, systematic manner to ensure that they meet the needs of, and satisfy the expectations of, the various stakeholders in the Sectoral Plan for Deep Geological Repositories. This is particularly the case for the regulator (ENSI), who will need to review the dose calculations as part of their overall assessment of Nagra's work for SGT Stage 2.

Management of calculations is a process that covers their planning (including goal setting) and execution, as well as the interpretation and documentation of results. It further includes the documentation of the modelling approaches and input data used, as well as the documentation of the various QA measures carried out.

The process involves two principal parties (Nagra and its contractor, AF-Consult Ltd.), each of whom have specific responsibilities for the decisions made and actions that are undertaken. Both parties make use of certain instruments, such as software tools and documents of various types, to facilitate the process.

The responsibilities of the principal parties and the specific activities and decisions assigned to them are described in Section B.1. Section B.2 outlines the software tools developed to facilitate the modelling work and specific quality assurance (QA) measures applied when developing and deploying these tools (QA is discussed in more general terms in Appendix C). Each of the tools is then described in more detail in Sections B.3 to B.5.

B.1 Overview of management process

The two principal parties involved in the modelling work are Nagra, which has overall responsibility for the management of calculations and for the use of the results, and its contractor, AF-Consult Ltd., which performs the calculations. The process of managing the calculations is presented in overview in Fig. B-1.

Nagra begins the process by defining the general modelling approach for all calculation cases to be analysed in SGT Stage 2, including the safety assessment codes to be used. The definition of the general modelling approach results from various preparatory activities, such as code testing, system analyses, sensitivity analyses, iterations with the geological synthesis group, external peer review and so forth. The general modelling approach, as described in Chapter 5 of this report, is first documented in a technical note together with other key points relevant to the work of the contractor. Then, the general modelling approach undergoes a Data Clearance Process that ensures that suitable and consistent concepts are used. The Data Clearance Process is described further in Appendix C.

The contractor checks that it is possible to implement the general modelling approach as specified in the technical note and may, at this stage (or earlier), make recommendations to Nagra to improve the proposed approach if any shortcomings are identified. Once the contractor is convinced that the approach can, indeed, be implemented as specified, it proceeds to build the necessary computational environment to carry out the calculations, or to confirm that a suitable environment already exists. This environment is set up on a contractor-owned high-performance Linux cluster, which can run the safety assessment codes and carry out the required post-processing in an automatic and efficient manner.

In the meanwhile, Nagra compiles a catalogue of the input data that it judges will be needed for all calculation cases in a series of technical notes. The input data are also subjected to data clearance, this time to ensure that suitable and consistent data are used. Furthermore, most of the input data are subject to external peer review.

Once the data are made available to it, the contractor must decide whether all data required for the analysis of all calculation cases have been provided and have been cleared. It informs Nagra of any deficiencies or omissions in the data and Nagra updates the input data catalogue as necessary. The input data are then organised in specific Excel workbooks (see Section B.3).

At a later stage, Nagra audits the contractor to verify that the code environment and the input data tables have been prepared as required by the quality assurances guidelines (see Appendix C). This represents the first control point in the process (indicated by a red diamond in Fig. B-1).

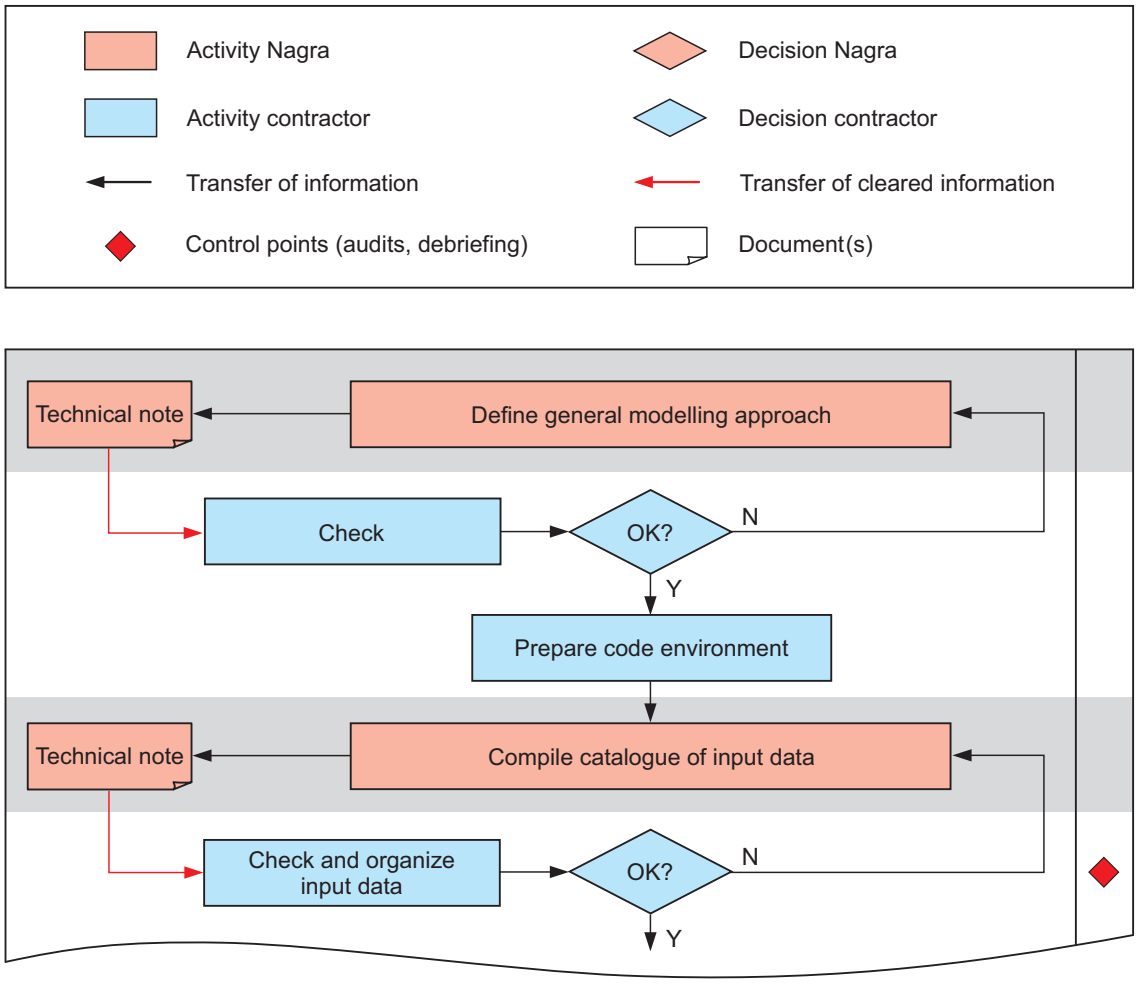


Fig. B-1: Overview of the calculation management process.

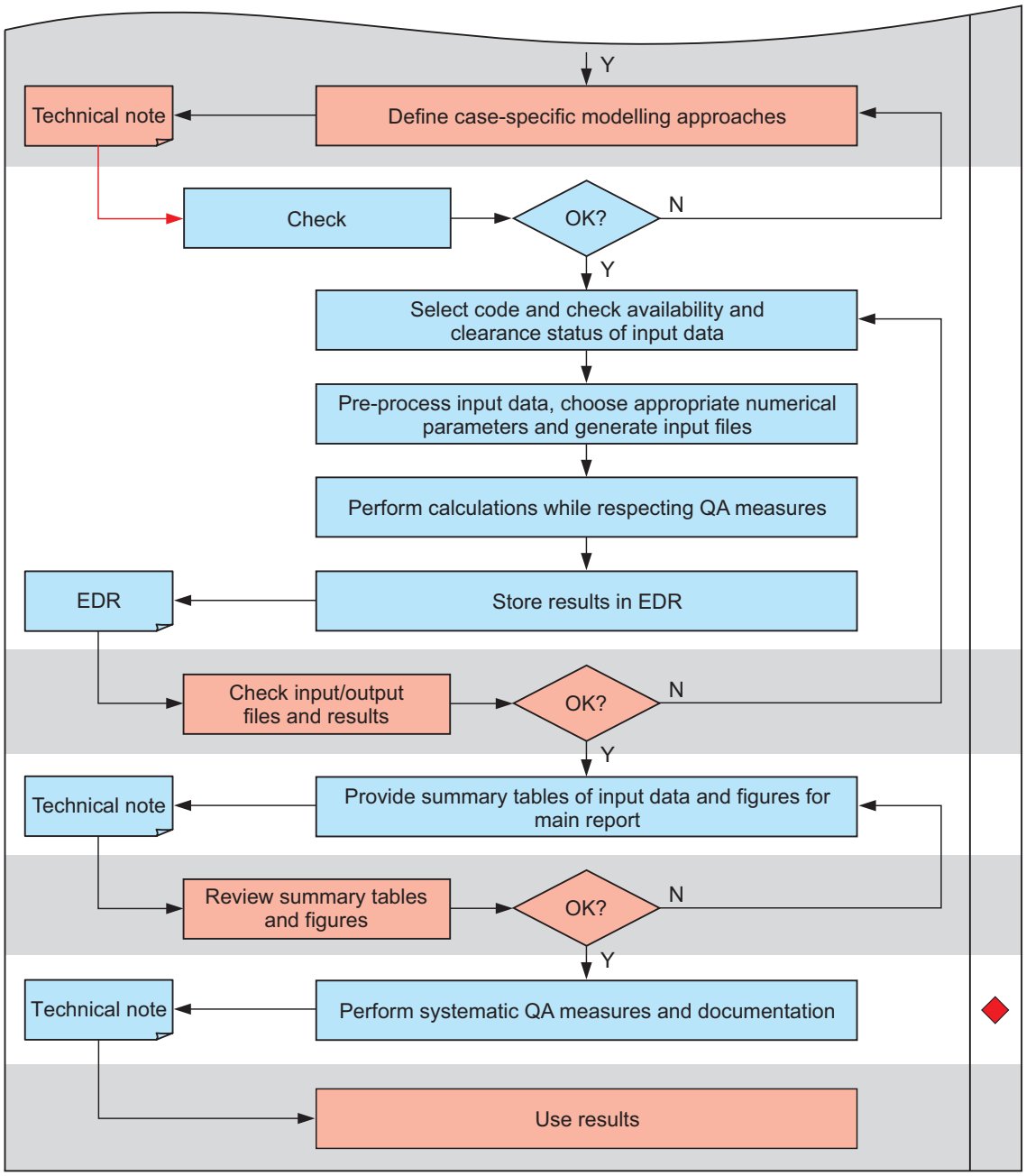


Fig. B-1: (continued)

Nagra also defines case-specific modelling approaches along with additional input data. These supplement the general modelling approach and the catalogue of input data for the calculation cases, thus providing the modelling details needed to implement each individual calculation case. In general, the case-specific modelling approaches and associated input data are fully documented in Nagra (2014b). As in the case of the general modelling approach and the catalogue of input data, they are also documented in technical notes together with key points relevant to the contractor, and undergo a data clearance procedure. The contractor checks that it can implement the case-specific modelling approaches as specified in the technical note and may make recommendations to Nagra to improve the proposed approach if any shortcomings are identified. Note that such recommendations can only refer to technical aspects of the case-specific modelling approach. Any difficulties encountered in implementing the case-specific modelling approach should not provide grounds for altering the calculation case definition itself.

Once the contractor has confirmed that the approach can, indeed, be implemented as specified, it proceeds with setting up the numerical model(s) to analyse the calculation case at hand. The contractor must ensure that it uses the latest quality assured version of each code (i.e. the code versions described in Chapter 3 and 4), and the contractor must also confirm that the input data it uses have been cleared by Nagra.

The contractor then builds the input files for the calculations, carries out any necessary pre-processing of input data (e.g. conversion of units), as well as any other preparatory work that may be needed. This includes, for instance, the setting of numerical parameter values and the generation of computational meshes. The next step is the execution of the calculations using specific tools (see Section B.4), while respecting the relevant quality assurance measures described in Appendix C, and storing the results and their associated input data in an electronic input data and results application (EDR, Nagra 2014d, see Section B.5)

The EDR gives Nagra direct access to the contractor's raw input and output files and provides figures and tables that summarise the key input data used and the results obtained. This allows the calculations to be checked by the Nagra staff responsible for generation and clearance of the general and case-specific modelling approaches, and by the Nagra staff responsible for input data. Nagra then needs to confirm that the modelling approaches and input data have been appropriately applied.

Once the calculations are complete, the contractor provides Nagra with figures and summary tables of input data and results in a short technical note. These figures and tables are directly added to Nagra (2014b) and to the overriding technical report for SGT Stage 2 (Nagra 2014a), while keeping editorial modifications at a minimum. Checks that the figures and tables added to these reports are consistent with the EDR are performed by Nagra staff. In addition, the summary tables of input data added to Nagra (2014b) are cross-checked with the corresponding tables in other reference reports as part of the technical documentation of SGT Stage 2. This approach ensures that consistent data is used throughout the safety assessment modelling process (see Section 2.1).

At the end of the modelling work, the contractor performs its own review of the work carried out. This includes further, systematic quality assurance measures that are enacted and documented by the contractor in a technical note.

Later, Nagra will again audit the contractor to verify that the calculations have been carried out as required by the quality assurances guidelines (see Appendix C). This will be combined with a debriefing meeting as required by the Nagra Quality Management System and forms the second control point in the calculation management process.

B.2 Overview of software tools and specific QA measures

Software tools

The large number of calculation cases, each of which involves the running of several computer codes, requires a system of software tools that enables the calculations to be executed and documented efficiently and in such a manner that all requirements regarding quality management are met (see Appendix C). Furthermore, such a system of software tools must be flexible enough to allow model runs to be revisited and modified if necessary. The system of software tools developed for this purpose is illustrated in Fig. B-2 and consists of:

- Excel workbooks, one for each of the main computer codes, each consisting of:
  - a database to manage the input data used in input files, including their clearances and references;
  - a table of calculation cases and model runs to select the individual sets of parameter values that make up the input files for a specific model run;
  - a pre-processor to automatically generate setup files[78], which are a first step in the creation of input files for the main codes, using the above mentioned database and the table of calculation cases and model runs;
  - a revision control system (RCS) to provide a continuous record of all setup files created.
- a job browser, which is used to generate the input files, to initiate calculations, to keep track of the current status of each calculation, to trace modifications in input files by communicating with the Revision Control System, and to create plots of key results;
- the EDR, which stores all input files, results and other model run data in an interactive electronic data base.

Detailed descriptions of each of these software tools are provided in the following sections.

[78] Setup files contain the basic structure of the model domain (e.g. the arrangement of transport paths). This structure may then be used for several calculation cases.

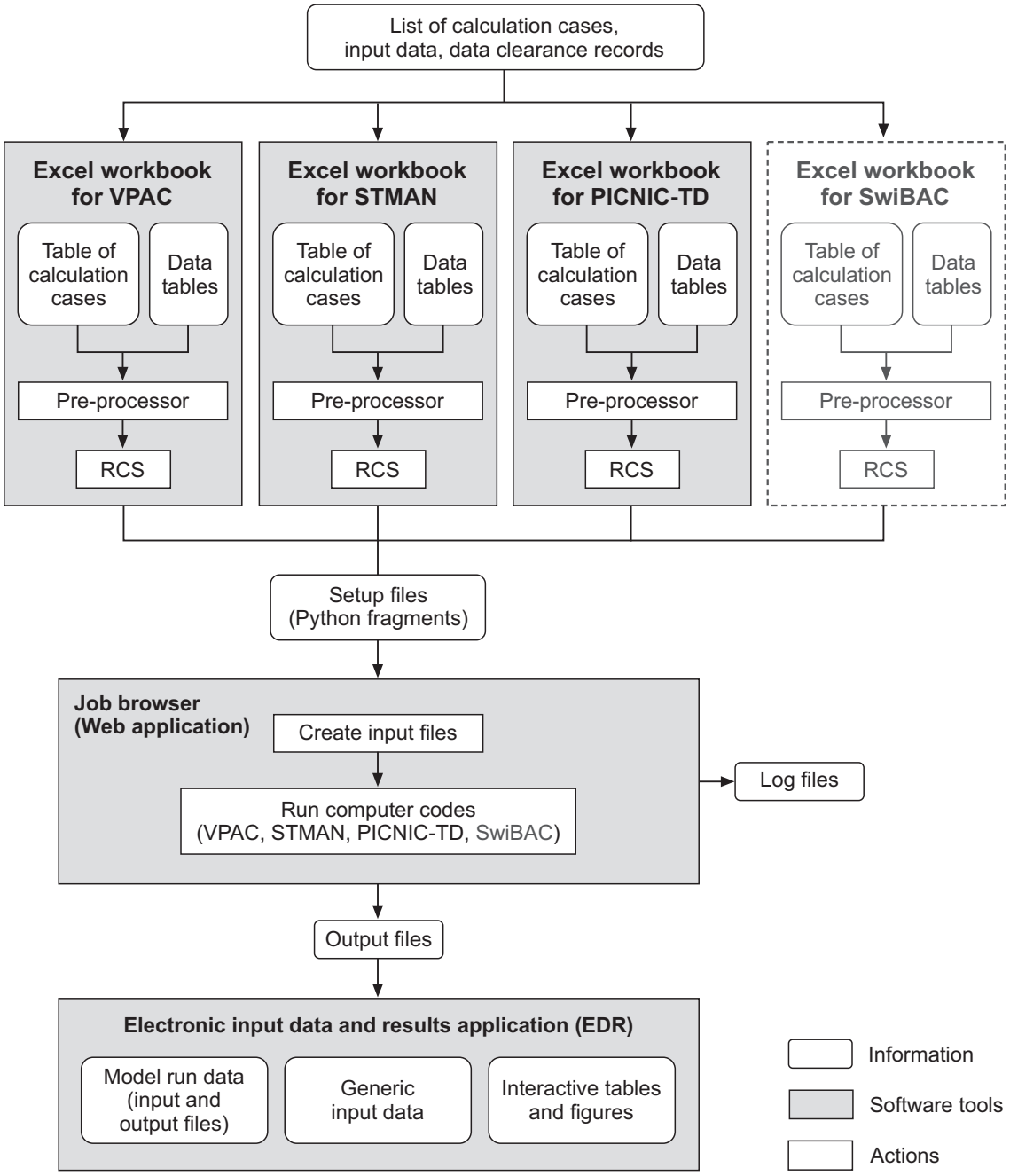


Fig. B-2: Overview of the system of software tools to manage the execution and documentation of calculation cases and individual model runs.

Note that an Excel workbook for SwiBAC has not been implemented for SGT Stage 2, since a set of generic BCDFs is used to convert radionuclide release from the geosphere into dose rates (see Section 4.1.8).

Specific QA measures

As part of quality management, the software tools and their communication pathways have themselves to be carefully checked. Thus, for example, the tables comprising the database in the Excel workbooks are verified by comparing the entries in the input data tables with the reference documents. Immediately after this verification step, the data in the input data tables are write-protected to avoid inadvertent modifications.

The setup file generation functionality of the Excel workbooks is verified (i) by QA of the Visual Basic Application used and (ii) by systematically checking whether the parameters in sample input files were identical to those in the corresponding input data tables. The second step also implicitly confirms that the job browser correctly merges the setup files into the input files. The tracking of the setup files with a revision control system (RCS) provides an additional QA step.

The EDR applies data operations to the results (e.g. extraction of maxima of time series) to generate figures and tables. These data operations are tested individually by performing unitary tests.

As described in Section 2.2, the calculated release of radionuclides from the near field provides the source term for the transport and retention modelling in the geosphere. The main output files from the main codes used for near-field modelling, STMAN and VPAC, which contain the time histories of nuclide releases from the near field are in the correct format to act as input files for the main code used for geosphere modelling, PICNIC-TD. PICNIC-TD also produces an output file in the correct format to be used directly as input to the biosphere code, SwiBAC, although SwiBAC does not use this type of input in the present dose calculations (see Section B.3 and Section 4.1.8). The lack of any need for reformatting of output files as input files for other codes eliminates a potential source of error in implementing the calculations.

A further quality check of individual and model-chain calculations is to verify whether the evolution of the total activity of each nuclide summed over all modelled components (e.g. all near-field and geosphere models), plus the activity that leaves the modelled barrier system, matches the total activity that should be globally present, taking into account radioactive decay and ingrowth.

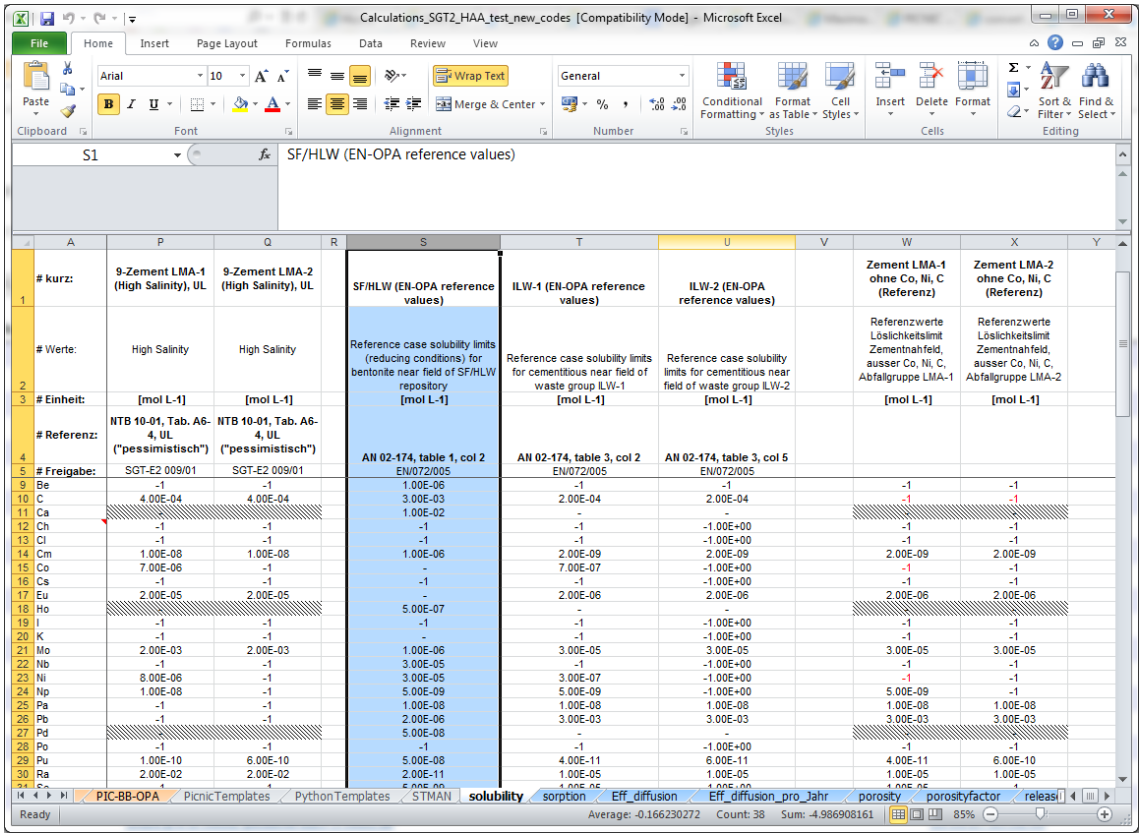
B.3 Excel workbooks

Three Excel workbooks are used, one for each of the near field and geosphere codes VPAC, STMAN and PICNIC-TD. There is currently no Excel workbook implemented for SwiBAC. This is because generic biosphere dose conversion factors (BDCFs) are used to convert geosphere release rates into dose rates (see Section 4.1.8). Each workbook consists of the following components.

(i) Database to manage input data for use in input files

The input files required by STMAN and PICNIC-TD (and also SwiBAC) are simple text files consisting of a series of sections or blocks. Each block starts with a unique title and ends with an end keyword. For example, the STMAN block enclosed between the keywords RELEASE and END holds release rates of radionuclides from the waste matrices as functions of time. The data required to construct such blocks are held in the data tables of the Excel workbook. For example, Fig. B-3 shows an excerpt of the table "solubility" with the element-dependent solubility limits for various chemical conditions. Starting from line 9, the solubility limits for the different elements are listed. Similarly, there are tables for sorption coefficients, inventories, release rates, decay constants etc., corresponding to the data blocks of an STMAN input file.

The VPAC input file format is a combination of text files with XML structure and, for information with high memory requirement, additional binary files. The VPAC XML file structure consists of several XML sub-files that contain all the information needed for the VPAC calculation (material properties, mesh information, chemical components, etc.). All these XML sub-files are generated by a single setup file, which contains all the required data. These data are obtained from the input data tables in Excel workbooks in the same manner as described above for STMAN and PICNIC-TD.



	A	P	Q	S	T	U	W	X
1	# kurz:	9-Zement LMA-1 (High Salinity), UL	9-Zement LMA-2 (High Salinity), UL	SF/HLW (EN-OPA reference values)	ILW-1 (EN-OPA reference values)	ILW-2 (EN-OPA reference values)	Zement LMA-1 ohne Co, Ni, C (Referenz)	Zement LMA-2 ohne Co, Ni, C (Referenz)
2	# Werte:	High Salinity	High Salinity	Reference case solubility limits (reducing conditions) for bentonite near field of SF/HLW repository	Reference case solubility limits for cementitious near field of waste group ILW-1	Reference case solubility limits for cementitious near field of waste group ILW-2	Referenzwerte Löslichkeitslimit Zementnahfeld, ausser Co, Ni, C, Abfallgruppe LMA-1	Referenzwerte Löslichkeitslimit Zementnahfeld, ausser Co, Ni, C, Abfallgruppe LMA-2
3	# Einheit:	[mol L-1]	[mol L-1]	[mol L-1]	[mol L-1]	[mol L-1]	[mol L-1]	[mol L-1]
4	# Referenz:	NTB 10-01, Tab. A6-4, UL ("pessimistisch")	NTB 10-01, Tab. A6-4, UL ("pessimistisch")	AN 02-174, table 1, col 2	AN 02-174, table 3, col 2	AN 02-174, table 3, col 5		
5	# Freigabe:	SGT-E2 009/01	SGT-E2 009/01	EN/072/005	EN/072/005	EN/072/005		
9	Be	-1	-1	1.00E-06	-1	-1	-1	-1
10	C	4.00E-04	4.00E-04	3.00E-03	2.00E-04	2.00E-04	-1	-1
11	Ca			1.00E-02	-	-		
12	Ch	-1	-1	-1	-1	-1.00E+00	-1	-1
13	Cl	-1	-1	-1	-1	-1.00E+00	-1	-1
14	Cm	1.00E-08	1.00E-08	1.00E-06	2.00E-09	2.00E-09	2.00E-09	2.00E-09
15	Co	7.00E-06	-1	-	7.00E-07	-1.00E+00	-1	-1
16	Cs	-1	-1	-1	-1	-1.00E+00	-1	-1
17	Eu	2.00E-05	2.00E-05	-	2.00E-06	2.00E-06	2.00E-06	2.00E-06
18	Ho			5.00E-07	-	-		
19	I	-1	-1	-1	-1	-1.00E+00	-1	-1
20	K	-1	-1	-	-1	-1.00E+00	-1	-1
21	Mo	2.00E-03	2.00E-03	1.00E-06	3.00E-05	3.00E-05	3.00E-05	3.00E-05
22	Nb	-1	-1	3.00E-05	-1	-1.00E+00	-1	-1
23	Ni	8.00E-06	-1	3.00E-05	3.00E-07	-1.00E+00	-1	-1
24	Np	1.00E-08	-1	5.00E-09	5.00E-09	-1.00E+00	5.00E-09	-1
25	Pa	-1	-1	1.00E-08	1.00E-08	1.00E-08	1.00E-08	1.00E-08
26	Pb	-1	-1	2.00E-06	3.00E-03	3.00E-03	3.00E-03	3.00E-03
27	Pd			5.00E-08	-	-		
28	Po	-1	-1	-1	-1	-1.00E+00	-1	-1
29	Pu	1.00E-10	6.00E-10	5.00E-08	4.00E-11	6.00E-11	4.00E-11	6.00E-10
30	Ra	2.00E-02	2.00E-02	2.00E-11	1.00E-05	1.00E-05	1.00E-05	1.00E-05

Fig. B-3: Excel workbook, showing the table "solubility", which lists element-specific solubility limits for various waste types and chemical conditions.

The element Ch denotes organic carbon, a value of -1 denotes unlimited solubility, and a hyphen means that no solubility limitation is accounted for.

Example from a preliminary version of the Excel workbook used for the present dose calculations.

(ii) Table of calculation cases and model runs

The table of calculation cases and model runs is used to define the set of input parameters for each calculation case and to generate the input files for VPAC, STMAN and PICNIC-TD. Each row of the table holds all data and links required to create a setup file. Fig. B-4 shows an excerpt of such a table for STMAN. Columns up to W (but not including A) are used to specify basic data required to identify a calculation case uniquely, e.g. by specifying the type of inventory (SF), the disposal canister type (BUO), which code and sub-code to be used for the calculation (STMAN, SPENT), as well as other supplementary information. The case name in Column A (e.g. HAA-pWG-OPA-stman-BE-6-BUO) is constructed automatically, based on a pre-defined naming convention for input files. Similar commands are used to construct the name of the input file and the title of the calculation case as it appears on the output plots. The text elements are taken primarily from cells in the same row of the table, thereby guaranteeing consistency between file names, titles and input data.

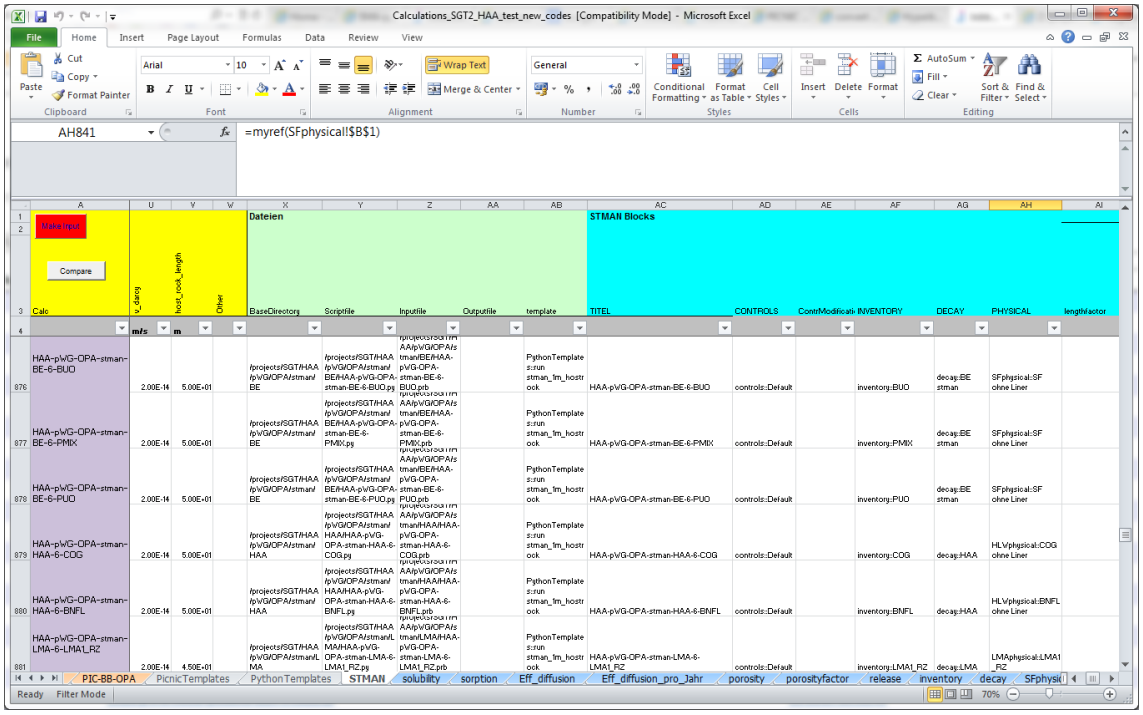


Fig. B-4: Excerpt from a table with calculations cases and model runs for STMAN, illustrating the definition of the names of individual calculation cases.

Example from a preliminary version of the Excel workbook used for the present dose calculations.

Fig. B-5 shows a different section of the same table as in Fig. B-4, defining the parameter sets for the various blocks of an input file. Instead of containing single data values, these cells contain links to other data tables and columns as required to define any particular calculation case. Each link has the structure "table name"::"column header". For example, for the calculation case HAA-pWG-OPA-stman-HAA-6-BNFL (row 880), the reference "solubility::Bentonit (reduzierend Referenz)" is a link to the column labelled "Bentonit (reduzierend Referenz)" in data table "solubility" (see Fig. B-3).

(iii) Pre-processor for automatic generation of setup files

In addition to the data tables and the calculation case table, the Excel workbook for each code also incorporates a macro, i.e. a program written in the MS Office programming language Visual Basic for Applications (VBA). This macro creates so-called setup files for VPAC, STMAN and PICNIC-TD. These setup files are later used by the job browser to construct complete input files (see below). The VBA macro is run from the table of calculation cases, where its execution is initiated by selecting any cell in the row of a particular calculation case and then by clicking on the red button labelled "Make Input" in the upper left-hand corner of the table.

The macro starts by creating a new file with the name and directory path specified in the column entitled "Inputfile". Then it writes introductory identifier lines and the title of the calculation case into that file, followed by a series of blocks, each consisting of the contents of the referenced column in one of the data tables. For QA purposes, the macro also conducts consistency checks and alerts are issued if inconsistencies are detected.

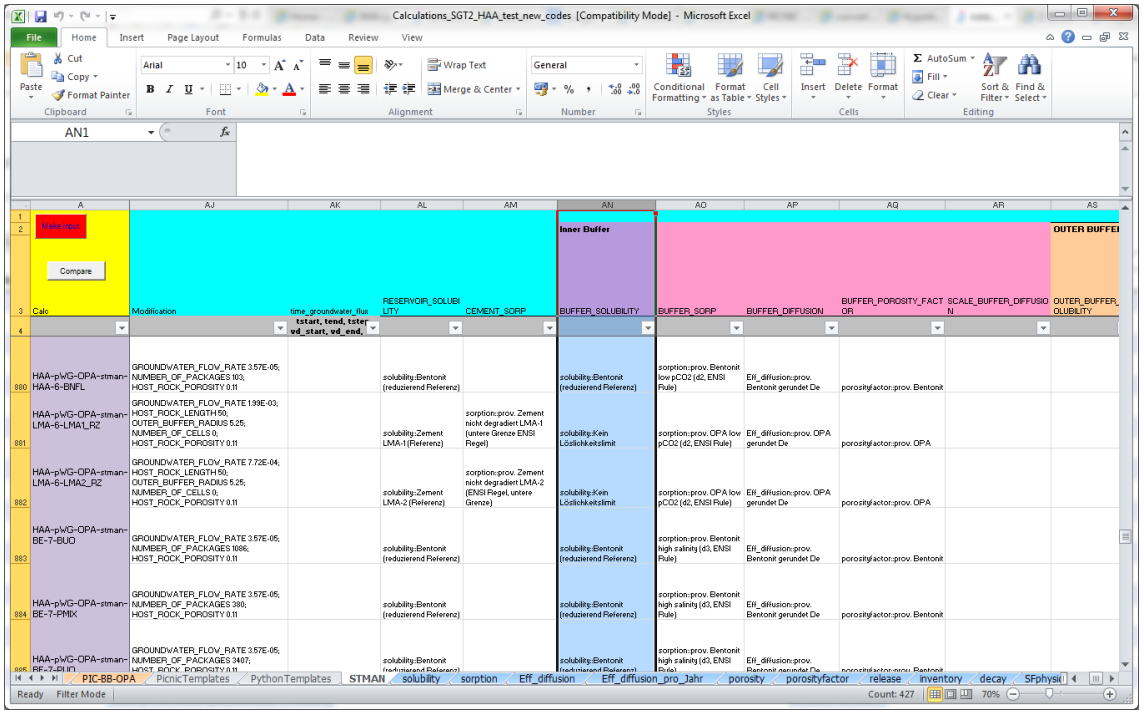


Fig. B-5: Excerpt from a table with calculations cases and model runs for STMAN, showing links to certain columns in the data tables as required for the creation of setup files.

Example from a preliminary version of the Excel workbook used for the present dose calculations.

(iv) Revision Control System

A setup file may be subject to modifications due to changes in model parameter values or as a result of errors being detected in the QA process. A widely used revision control system, named RCS, is used to keep track of all changes made to the setup files over the course of time.

The RCS manages multiple revisions of files and automates the storing, retrieval, logging and identification of revisions. The RCS is most useful for text that is revised frequently, such as computer codes and documentation. The basic user interface is simple. The command "ci", short for "check in", puts the contents of a file into an archive file, also called an RCS file. An RCS file contains all revisions of a particular file. The command "co", short for "check out", retrieves a revision from an RCS file. The complete reference material for the freely available RCS can be found on the internet. The RCS functionalities used by the Excel Workbooks are:

- Store and retrieve multiple revisions of setup files: RCS saves all old revisions in a memory saving way. Changes do not destroy the original and previous revisions. Thus, they remain accessible. Revisions can be retrieved according to revision numbers, symbolic names, dates and authors.
- Maintain a complete history of changes: RCS logs all changes automatically. Besides the text of each revision, RCS stores the author, the date and time of check-in, and a log message summarising the change. The logging facilitates control of the history of a setup file.
- Automatically identify each revision with name, revision number, creation time, author, etc. The identification is like a stamp that can be embedded at an appropriate place in the text of a revision. The identification facilitates the controlled use of revisions.
- Compare different versions of a file.

Fig. B-6 shows the column called "Date Revision" in an Excel workbook that lists the date and the time of check-in and the revision number. This column is updated by pressing the button "Make Input". Therefore, if some changes are made in the data, the system asks for a log message to indicate that changes have been made. Once the message is typed in the column "logmessage", the column "Date Revision" is updated and a new revision is stored in the RCS.

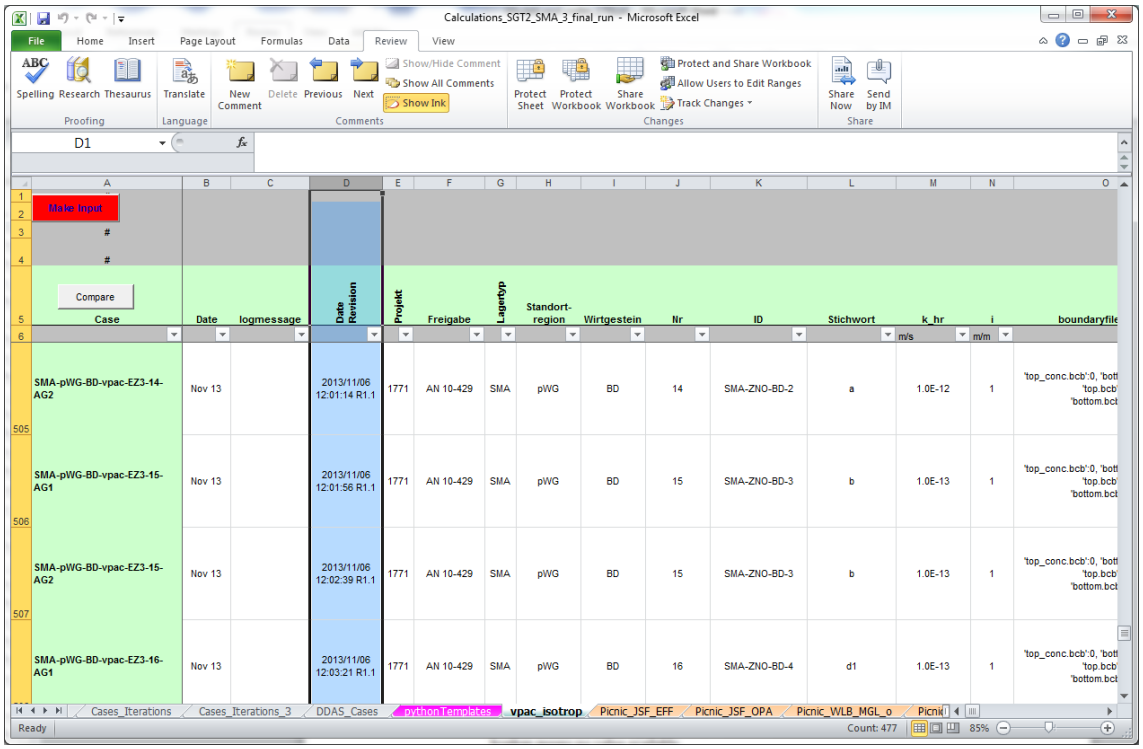


Fig. B-6: Excel workbook, showing the column "Date Revision", which lists date and time of check-in and the revision number.

Example from a preliminary version of the Excel workbook used for the present dose calculations.

B.4 Job browser

The job browser is a web application created with a python script. It allows the execution of the codes VPAC, STMAN and PICNIC-TD and the generation of the required input files. At the same time, the job browser provides information about the available input files and their status. An example screenshot of the job browser is given in Fig. B-7.

To start a job or to retrieve information about a running or finished job, first a job type is selected at the top of the main window of the job browser. These job types are, e.g., creating input files for VPAC, STMAN and PICNIC-TD using the setup files mentioned in the previous section, or running the codes. The two input fields ("Path(s)" and "Search") are used to select a directory in which files may be searched for a specified character pattern. By clicking on the button "Go", the job browser searches for jobs that correspond to the selected job types and displays the jobs matching the specified character pattern. The user can also select a toggle button to the right of the input "Path(s)" to show which jobs have finished successfully.

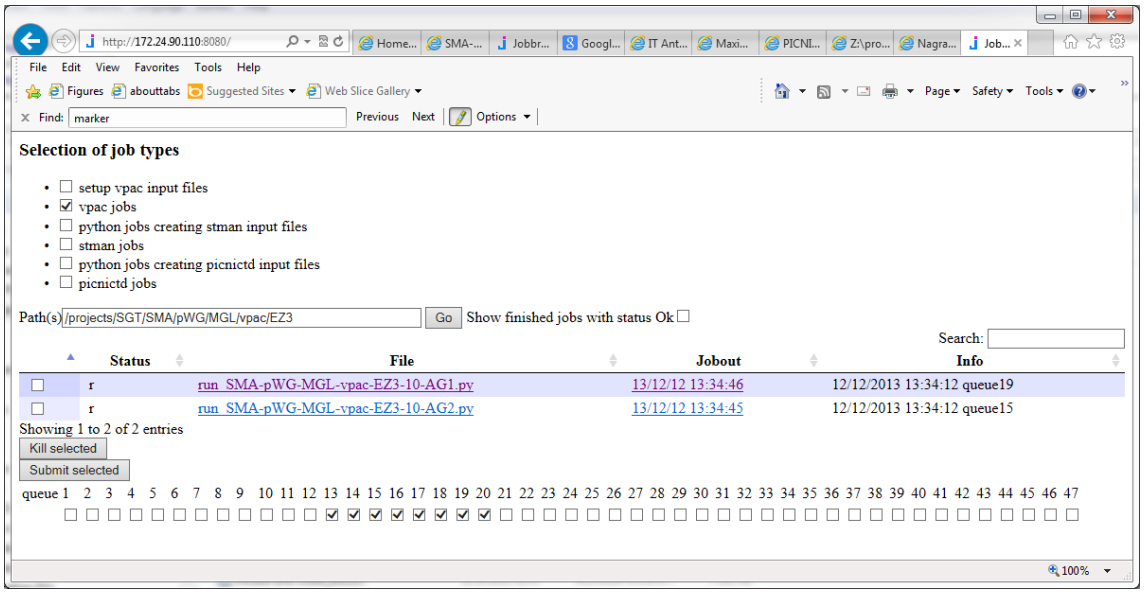


Fig. B-7: Example of the interactive window of the job browser.

The displayed information about the jobs and the available operations below the "Path(s)" input are:

- The column "Status" shows the current status of jobs (e.g., 'r' means running, 'e' means error, 'qw' means job waiting in the queue, 't' means a transition state, e.g. during job start).[79]
- The column "File" shows the jobs (e.g. input files). The content of an input file can be shown by simply clicking on the file link.
- The column "Jobout" shows the last time at which the output file was updated. The last few lines of the output file can be displayed by simply clicking on the link.
- When a job has been submitted and is in the process of being executed, the information about the time at which the job was started and the queue (node) number of the Linux cluster at which the job is running are displayed in the column "Info".

Running jobs can be killed (stopped) at any time by selecting the corresponding switches and pressing the button "Kill selected". All switches to the left can be selected manually. Selected jobs can be submitted by pressing the button "Submit selected". The last line shows the queues (nodes) on the Linux cluster that are currently available for job submission.

[79] Note that, when modifying an input file but keeping an existing name, the job browser recognises the modification and the status becomes "o" (old, with a message about the modification, e.g. "source term is newer than …"); see the description of the revision control system.

B.5 Electronic input data and results application (EDR)

The EDR (Nagra 2014d) stores all input files, output files and post-processed results. Together with a couple of interactive features, it provides a convenient platform for the discussion and verification of results. A typical screenshot of the EDR is shown in Fig. B-8.

The EDR provides full flexibility to create any graph of radionuclide fluxes as functions of time or bar plots with maximum radionuclide fluxes from the stored results. Various options allow different calculation cases or different transport paths to be selected. The radionuclide fluxes may be plotted in units of activity, moles or effective dose rates (in which case the EDR multiplies calculated fluxes by the BCDFs).

The EDR further allows a one-by-one comparison of input files, thus facilitating a quick understanding of differences between results. Finally, the generated figures and tables may be exported for use in reports or further analyses.

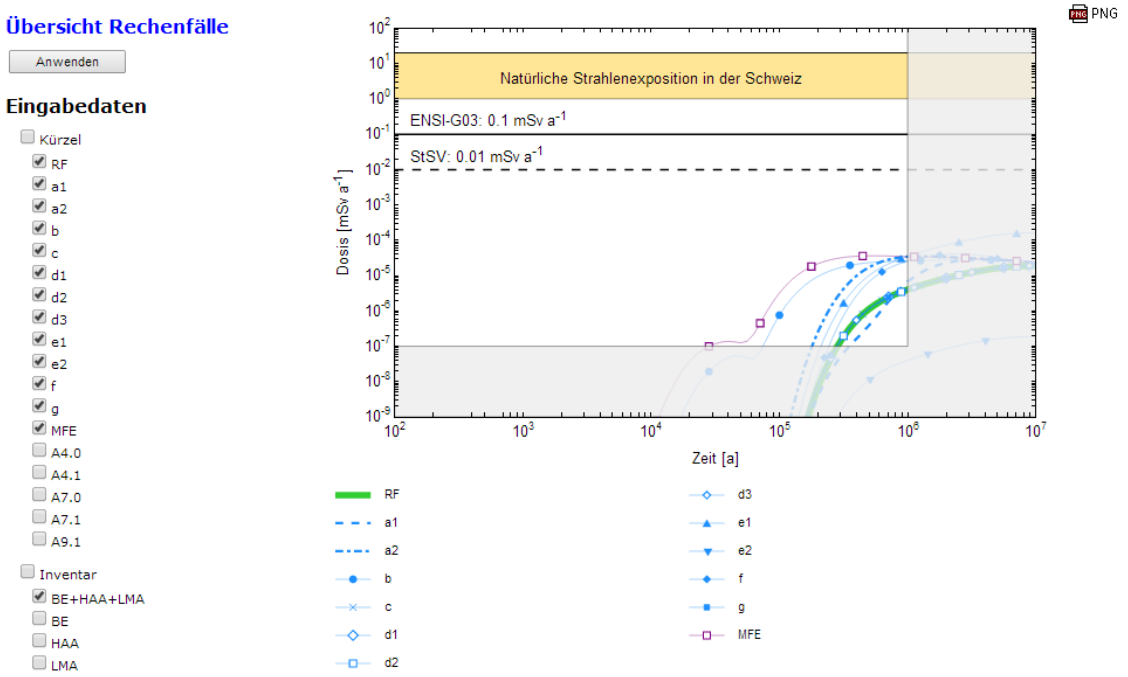


Fig. B-8: Typical screenshot of the EDR, displaying calculated dose rates as functions of time.

Example from a preliminary version of the EDR for the present dose calculations.

C Quality Assurance

The dose calculations for the provisional safety analyses and the corresponding preparatory work are conducted as a sub-project of the main project "Provisional Safety Analyses for SGT Stage 2", both of which are carried out in compliance with the Nagra Quality Management System (QMS). The QMS defines specific working procedures that may include general quality assurance measures, e.g. external peer review, as well as quality assurance measures specific to individual activities. Such specific measures are documented in quality assurance guidelines. There are four quality assurance guidelines that refer to safety assessment modelling.[80]

Use of computer codes for safety analysis

The adequacy of the safety assessment codes for the different calculation cases and the modelling approaches adopted needs to be checked (explicit / implicit consideration of processes and parameters, acceptable simplifications) and the codes need to be verified to the extent required by the modelled problem (see Section 2.3). Attention has to be given to the systematic naming and structuring of the assessment cases and the corresponding input and output files. Input data need to be traced to, and checked against, their source and, if relevant, to the corresponding data clearance. Version control has to be implemented for all programs, scripts and input files, and log files with specific information on the execution of each calculation case must be created. QA measures, such as consistency checks of input and calculated data, must be carried out and may be integrated into the log file. Automatic control measures both at code execution and post-processing of results have to be carried out. QA measures must be documented in technical notes and added to the QA documentation of the project.

Test procedures for safety analysis modelling

The test procedures include the checking of conceptual models, of mathematical models (e.g. equations, initial and boundary conditions), of numerical solution techniques, of input data and of results and arguments. It involves plausibility checks (e.g. comparison with information from other post-closure safety assessment studies and comparison with results from other analyses or other calculation cases) and can additionally require independent calculations (simplified or equally complex), considerations based on the same method and / or the same modelling approach, or – in an extreme case – a calculation with a different method or considerations based on a different modelling approach. It may also involve tests of convergence of the solution as discretisation in space and time is refined (solution verification).

Input data need to be traced to, and checked against, their source (see above) and summary tables of input data are generated for back-checking with project managers responsible for the original source data. The basic checks must always be done by the person that has done the modelling work. According to the relevance of the results, other persons from the same organisation that has carried out the modelling work and / or from other organisations (including Nagra) may do the same or different checks independently. Special care is required for tasks that are known to be critical. Quality assurance measures must be documented in technical notes and added to the QA documentation of the project.

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[80] This is consistent with the requirements specified in ENSI (2009a), according to which "quality assurance measures for handling data and performing quantitative or qualitative analyses as part of the safety assessments have to be put in place and documented".

Acquisition and development of safety analysis codes

This guideline specifies the principal requirements on, and quality assurance measures for, safety analysis codes. All computer codes used in post-closure safety analysis have been developed specifically for Nagra; other, commercially available codes are not currently used. Requirements on specifically developed codes include clear program architecture, use of an established programming language, clear structuring and annotation and good prospects for active maintenance and support. A verification plan must be defined before implementation and the source code must be peer reviewed within the development team. Verification with at least one other well-established code or with analytical solutions for selected cases is mandatory and verification exercises with calculations undertaken by other organisations are desirable; e.g. within the framework of international benchmark studies (the topic of code verification is discussed in Section 2.3). Documentation should include descriptions of the area of application, the conceptual and mathematical models and the FEPs included, program architecture, solution methods and hardware requirements. A program-specific logbook has to be opened and errors detected in the computer program must be recorded therein (see above).

Maintenance of computer codes for safety analysis

For each safety assessment code, a log-book is maintained in which quality assurance measures and their results are recorded, together with other relevant information, such as the person responsible for the code, its area of application, the supplier / developer, available documentation, the current program version and the computational environment.

Quality assurance measures are adopted to ensure the operational readiness of the compiled version of a code and its computational environment (including pre- and post-processing) for safety analysis. These include specific checks that are undertaken when the code has been modified (e.g. adaptations to new computer system) or when modifications e.g. to the input / output procedures have been made. The checks are usually performed using the defined standard calculations for verification (also after reinstallation or recompilation). Version control is implemented for all program files.

Documentation

All QA-measures that are carried out under these guidelines have to be documented. The documentation is assessed in regular audits at the organisation which is in charge of the modelling work; see also Appendix B.

D Symbols and Abbreviations

This chapter lists the most important symbols and all the abbreviations used in the present report and shows the links between individual model parameters and the processes and parameters relevant to long-term safety, as given in Appendix A.

D.1 Main symbols used in concepts and modelling approaches for the engineered and geological barriers

Symbol	Explanation and remarks	Relevant process or parameter
A	cross-sectional area of 1D transport path in the geosphere	
A_0	initial total (inner and outer) surface area of fragmented glass block	
B	half-distance between planar, transmissive elements ($(B-b)$ is the thickness of the diffusion-accessible rock matrix).	
B	parent nuclide	
BM	buffer medium	
b	half-aperture of discrete water-conducting feature	
c	concentration	
c_l	concentration in aqueous phase	
c_{GW}^N	nuclide concentration in incoming groundwater (STMAN)	
c_s	concentration in solid phase	
c_{sol}^E	solubility limit for element E	PT-3
$\boldsymbol{D}$	hydrodynamic dispersion tensor	
D_p, D_p^E	pore diffusion coefficient (for element E)	PT-5, PG-22
$DP^{N,E}$	rate of dissolution / precipitation of nuclide N, which is an isotope of element E	
d	separation distance between emplacement rooms	
E, $\tilde{E}$	element E, element $\tilde{E}$	
f	hydraulic source term	
f_m	fractional release rate from waste matrix type m	PT-2
f_{GW}^N	nuclide flux of incoming groundwater (STMAN)	
G	total nuclide release rate	
g	gravitational acceleration	
h	hydraulic head	
h	height of emplacement room	
h_d	spatial discretisation	
IRF	(initial) instant release fraction	
I, I_m	total inventory, inventory of waste matrix type m	
i, i_v	hydraulic gradient, vertical hydraulic gradient	PT-5, PG-6, PG-7, PG-8

Symbol	Explanation and remarks	Relevant process or parameter
K, $\boldsymbol{K}$, K_h, K_v	hydraulic conductivity (tensor), horizontal hydraulic conductivity, vertical hydraulic conductivity	PT-5, PG-6, PG-7, PG-8
K_d^E	linear sorption coefficient for element E	PT-4, PG-21
k	corrosion rate, dissolution rate	
L	length of emplacement room / area	
L_c	length of disposal canister	
l, L_h	length of (horizontal) transport path	PG-13
m	thickness of rock unit	
N	nuclide	
N_{IRF}^N, N_m^N	total of instantly released inventory of nuclide N, gradually released inventory of nuclide N (in matrix type m)	
n	number of emplacement rooms within emplacement area	
$\vec{n}$	vector normal to model boundary	
n_s	number of equivalent glass spheres	
n^E	accessible porosity factor for element E	
P	concentration in discrete water-conducting feature	
Pe	Peclet number	
p	pressure in aqueous phase	
q	Darcy velocity	
q_L	Darcy velocity in discrete water-conducting feature	
Q	groundwater flow rate	
R^E	retardation coefficient for element E	
R_L	retardation coefficient in discrete water-conducting feature	
r	coordinate in radial direction	
r	specific corrosion rate, specific dissolution rate	
r_s	radius of equivalent glass spheres or waste matrix fragments	
r_0	radius of disposal canister	
r_0	initial diameter of waste form	
S_s	specific storage coefficient	
T	transmissivity of discrete water-conducting feature	PG-14, PG-8 (PG-6, PG-7, PG-8, PG-9)
$T_{1/2}$	half-life	
t_0	reference time for radionuclide inventory, start of time frame for safety assessment	
t_c	period of complete containment, time of canister breaching, time of instant release	PT-1
u	average linear velocity in the pore space	
V_m	volume of waste matrix type m	
V_R	volume of the "reservoir" used in the near-field models	

Symbol	Explanation and remarks	Relevant process or parameter
V_0	initial total volume of glass block	
W	total width of emplacement area	
w	width of emplacement room	
w_c	flow capture width	
Y	sink term to surrounding buffer medium (bentonite)	
z	coordinate in vertical direction	
α_L, α_T	longitudinal dispersion length, transversal dispersion length	
γ	rate of radioactive decay and ingrowth	
δ_L	specific surface area of discrete water-conducting feature (area of surface per unit volume of water)	
ε	total porosity	
ε^E	element-specific porosity	PG-10
ε_L	porosity in discrete water-conducting feature	
λ, λ^N	decay constant (for radionuclide N)	
ρ	density	
ρ_s	dry bulk density of solid material	
ρ_{grain}	(average) grain density of solid material	
σ^{BN}	branching ratio for the decay of parent B into daughter N	
σ	numerical parameter in VPAC	
τ	lifetime	
Θ	source / sink term	

In general, any consistent set of units may be used for modelling water flow and radionuclide transport in the engineered and geological barriers. Thus, in this report:

L denotes a unit of length;

T denotes a unit of time; and

M denotes a unit of mass.

As an exception, the code VPAC requires that the parameter values in the input files be given in the units expected by the code. These default units are given in Tab. 3-2. STMAN and PICNIC-TD allow the user a choice of units, which are then converted by the codes into the expected internal units.

D.2 Main symbols used in concepts and modelling approaches for the biosphere

Symbol	Explanation and remarks	Relevant process or parameter
For abbreviations of compartments, see Tab. 4-1		
A	surface (plan) area of a compartment	
D	diffusive flux	
D_0	diffusion coefficient in free water	
D_p	effective dose for exposure pathway p	
E_p	exposure factor for exposure pathway p	
F	water flux	PG-31
H_{exp}	dose coefficient for exposure mode "exp"	
K_d	solid / liquid distribution coefficient	
l	depth / thickness of a compartment	
M	parent radionuclide	
M	solid material flux	
N	radionuclide	
P_p	processing factor that converts an inventory into a concentration for exposure pathway p	
S	external radionuclide source	
s	area scaling factor	
T	tortuosity	
ε	porosity	
λ_{ij}	fractional transfer rate from compartment i to compartment j	
λ, λ^N	decay constant (for radionuclide N)	
ρ	solid dry density	
σ^{MN}	branching ratio for the decay of parent M into daughter N	
θ	volumetric moisture content	

In general, any consistent set of units may be used for biosphere modelling. Thus, in this report:

L denotes a unit of length;

T denotes a unit of time; and

M denotes a unit of mass.

Bq denotes a unit of radioactivity

Sv denotes a unit of radiological effective dose

SwiBAC allows the user a choice of units, which are then converted by the code into the expected internal units.

D.3 Abbreviations and code names

Abbreviation	Explanation and remarks
1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
AMBER	compartment modelling tool
ATA	alpha-toxic waste
BDCF	biosphere dose conversion factor
BIOPROTA	Biosphere modelling for waste repositories (collaborative project)
C++	programming language
CSA	cross-sectional area of a 1D transport path in the geosphere
DYLAN	differential-algebraic equation solver
ECZ, EG	effective containment zone (In German: "einschlusswirksamer Gebirgsbereich")
EDR	electronic input data and results application
EDZ	excavation damage zone
ENSI	Swiss Federal Nuclear Safety Inspectorate
FA	(spent) fuel assembly
FD	finite difference method
FE	finite element method
FEP	feature, event and process
FORTRAN	scientific programming language
GEOTRAN-2D	code for solute transport in a fractured porous medium
HLW	(vitrified) high-level waste
HPM	homogeneous porous medium
IAEA	International Atomic Energy Agency
ICRP	International Commission on Radiological Protection
ILW	intermediate-level waste
IRF	instant release fraction
J	junction (of transport paths in PICNIC)
KEG	Nuclear Energy Law (In German: "Kernenergiegesetz")
KNE	Commission on Nuclear Disposal (In German: "Kommission Nukleare Entsorgung")
KNS	Federal Nuclear Safety Commission (In German: "Eidgenössische Kommission für nukleare Sicherheit")
K06, K09	types of emplacement room for ILW and LLW
L	leg (transport path in PICNIC)
L/ILW	low- and intermediate-level waste
LLW	low-level waste
MIRAM	modelled inventory of Swiss radioactive materials
MODARIA	Modelling and Data for Radiological Impact Assessments (IAEA project)

Abbreviation	Explanation and remarks
MHFEM	mixed-hybrid finite element method (used in VPAC)
Nagra	National Cooperative for the Disposal of Radioactive Waste (In German: "Nationale Genossenschaft für die Lagerung radioaktiver Abfälle")
OECD/NEA	Organisation for Economic Co-operation and Development / Nulear Energy Agency
NC14M	Nagra C-14 model for the biosphere
PAGODA	integrated performance assessment tool
PG	process / parameter related to the geological barriers
PICNIC, PICNIC-TD	transport code for the geosphere (see Section 3.5)
PT	process / parameter related to the engineered barriers
QA	quality assurance
QM, QMS	quality management, quality management system
R	result
RCS	revision control system (software application)
REV	representative elementary volume
S	source term
SEFTRAN	2D finite element code for solute transport
SF	spent fuel
SGT	Sectoral Plan for Deep Geological Repositories (In German: "Sachplan geologische Tiefenlager")
SPENT (SP)	computer code used for near-field modelling (see Section 3.4)
SQE	software qualitiy engineering
STALLION (SN)	computer code used for near-field modelling (see Section 3.4)
STMAN	family of computer codes used for near-field modelling (see Section 3.4)
STRENG (SG)	computer code used for near-field modelling (see Section 3.4)
SwiBAC	Swiss Biosphere Assessment Code (see Section 4.3)
TAME	Terrestrial-Aquatic Model of the Environment (predecessor code to SwiBAC)
URL	underground research laboratory
VBA	Visual Basic for Applications
VPAC	Versatile Performance Assessment Code (see Section 3.3)
WLB	geological siting region Wellenberg
XML	extensible markup language