



Working Report 2012-06

Modelling Strategy Report

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ABSTRACT

This report presents a preliminary plan for the development and application of models for the probabilistic sensitivity analyses and the deterministic calculation cases that will be used to analyse scenarios in the 2012 safety case. The plan addresses both groundwater flow modelling and radionuclide transport modelling, primarily of the repository near field and of the geosphere. It also addresses the measures that will be applied during the implementation and documentation of the calculations that will contribute to the quality assurance of the safety case. It is expected that this plan will be refined and amended as experience is gained during the carrying out of the work.

Keywords: Safety case, Radionuclide transport, Near field, Far field, Activity release rates, Dose assessment, Connectflow, MARFA, Goldsim, FTRANS, REPCOM.

RADIONUKLIDIEN KULKEUTUMISMALLINNUKSEN STRATEGIA KALLIOPERÄSSÄ

TIIVISTELMÄ

Tämä raportti esittää suunnitelman todennäköisyyspohjaisten herkkyysanalyysien ja determinististen laskentatapausten kehittamisestä ja soveltamisesta skenaarioiden analysointiin vuoden 2012 turvallisuusperustelua varten. Suunnitelma käsittää sekä pohjaveden virtausmallinnuksen että radionuklidien kulkeutumismallinnuksen pääasiassa lähialueessa ja kallioperässä. Se käsittelee myös menettelyitä, joita käytetään käytännön laskennassa ja siihen liittyvässä dokumentoinnissa ja jotka tukevat turvallisuusperustelun laadunvarmistusta. On odotettavissa, että suunnitelma kehittyy edelleen käytännön kokemuksen myötä.

Avainsanat: Turvallisuusperustelu, Radionuklidien kulkeutuminen, Lähialue, Kaukoalue, Päästöaktiivisuusnopeus, Säteilyannosarviointi, Connectflow, MARFA, Goldsim, FTRANS; REPCOM.

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1 INTRODUCTION

1.1 Scope of this document

In the 2012 safety case, the fate of radionuclides in scenarios involving canister failure and radionuclide release will be analysed using a chain of models, with information flows between them, as illustrated in Fig. 1-1.

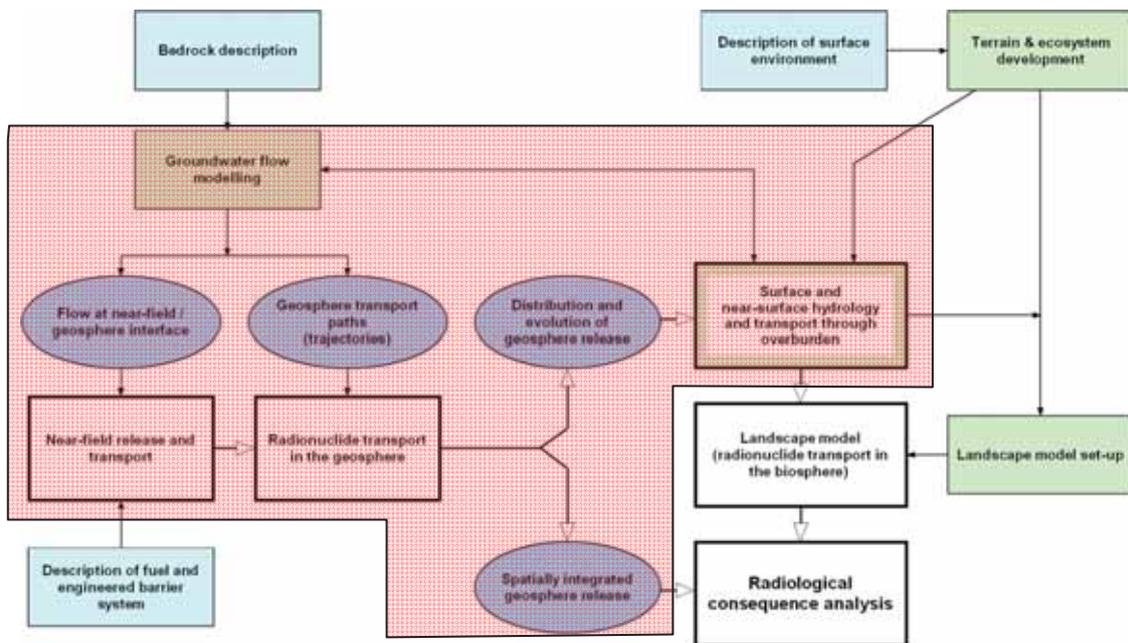


Figure 1-1. Models and information flows. Radionuclide release and transport models and consequence analysis are shown in white boxes. System descriptions are shown in light blue boxes, key supporting models in green boxes and their principal outputs in dark blue ovals. The shaded red area shows those models and information flows that are the subject of this document.

In agreement with most safety analysis carried out internationally, near-field release and transport modelling, geosphere transport modelling, biosphere transport modelling and radiological consequence analysis will be carried out sequentially. The present report focuses on near-field release and transport modelling, on the modelling of transport through the geosphere and overburden and on the detailed hydrogeological modelling that supports them, i.e. the shaded red area in Fig. 1-1. The report deals with the development and application of models in probabilistic sensitivity analysis to parameter variations and in the deterministic consequence analysis of calculation cases for each scenario. More details of the approaches to probabilistic sensitivity analysis and to the analysis of deterministic calculation cases will be given in the Analysis of Scenarios Report of the Safety Case portfolio (under development).

1.2 Regulatory background

Different regulatory requirements on the radiological protection are given in the Government Decree on the safety of disposal of nuclear waste (GD 736/2008) and in the

Finnish regulatory Guide YVL D.5 for different time windows. In the earliest time window, for a period that shall extend at a minimum over several millennia, Section 4 of DG 736/2008 states:

“The annual dose to the most exposed people shall remain below the value of 0.1 mSv.

and

“The average annual doses to people shall remain insignificantly low”.

In the longer term, the quantitative regulatory criteria relate directly to the release rates of radionuclides from the geosphere to the “living environment” (“geo-bio fluxes”). According to Guide YVL D.5,

Para. 3.14

“The sum of the ratios between the nuclide specific activity releases and the respective constraints shall be less than one”.

Guide YVL D.5 also contains a number of statements that have a direct bearing on the modelling of scenarios, and thus guide the present strategy. These statements relate to the need for the analysis as a whole not to overestimate or underestimate the performance of safety functions or to underestimate radiological consequences:

Para. A1.6

Simplifications of the models and the determination of the required input data shall be based on the principle that the performance of a safety function will not be overestimated while neither overly underestimated.

Para. A1.8

Selection of the computational methods and input data shall be based on principle that the actual radiation exposures or quantities of released radioactive substances shall with high degree of certainty be lower than those obtained through safety analyses. The uncertainties included in the safety analysis shall be assessed by means of appropriate methods, e.g. by sensitivity analyses or probabilistic methods.

There is also a statement regarding the need for stochastic modelling:

Para. A1.8

Whenever the input data used in modelling involve random variations due to e.g. heterogeneity of rock, stochastic models may be employed.

Finally, there is a statement regarding the documentation of calculations:

Para. A1.10

The safety shall be documented carefully. ... Another goal shall be traceability, implying that the justifications for the used assumptions, input data and models shall be easily found in the documentation.

These regulatory statements are referred to where appropriate throughout the present document.

1.3 Document structure

The remainder of this document is structured as follows:

- Chapter 2 describes the types of scenarios to be addressed in the 2012 safety case, and the broad approaches to their analysis.
- Chapter 3 describes the models and computer codes used for groundwater flow modelling.
- Chapter 4 describes the models and computer codes used to assess the release and transport of radionuclides.
- Chapter 5 concerns the application of models and computer codes in probabilistic sensitivity analysis.
- Chapter 6 concerns the application of models and computer codes in the analysis of scenarios for which a dose assessment is made.
- Chapter 7 concerns the application of models and computer codes in the analysis of other scenarios.
- Chapter 8 addresses probabilistic consequence analysis.
- Finally, Chapter 9 addresses the implementation and documentation of calculation cases, including the quality measures to be enacted.

The terms radionuclide transport processes and transport modelling are used in this document to refer to processes in, and modelling of, the repository near field, the geosphere (i.e. the repository system) and at the interface between the repository system and the surface system. Radionuclide transport processes also occur in the various ecosystems in the biosphere. These, however, are largely outside the scope of the present document.

2 SCENARIOS AND APPROACH TO THEIR ANALYSIS

2.1 Categories of scenarios

Following the Finnish regulatory guidelines given in YVL Guide D.5 (STUK 2009), three “top level” type of scenarios need to be considered in Posiva’s safety case: a base scenario, variant scenarios, and disturbance scenarios (Fig. 2-1).



Figure 2-1. Scenario classification according to YVL Guide D.5 (STUK 2009).

Appendix 1 of YVL-Guide D.5 provides the definitions of these scenarios:

- Base scenario: The base scenario shall assume the performance targets for each safety function, taking into account of incidental deviations from target values.
- Variant scenarios: The influence of declined performance of a single safety function or, in case of coupling between safety functions, the combined effects of declined performance of more than one safety functions shall be analysed by means of variant scenarios.
- Disturbance scenarios: Disturbance scenarios shall be constructed for the analysis of unlikely events impairing long-term safety.

The formulation of scenarios in the 2012 safety case will take as its starting point a base scenario, in which it is assumed that the target state defined for the repository system is achieved and in which the safety functions of system components are maintained in the long-term. Lines of evolutions will then be defined, and scoping calculations carried out when deemed necessary, to analyse the behaviour of the system or of parts of the system. If the scoping calculations show that the failure of one or more barriers (i.e. the failure of one or more safety functions) gives place to radionuclide releases, then this line of evolution will be included into variant or disturbance scenarios depending on the plausibility of the assumptions.

Those lines of evolution in which the containment safety function of the canister is maintained in the long term are included in the base scenario. Other lines of evolution in which the containment safety function of the canister could be compromised and that cannot be shown to be unlikely and are included in a set of variant scenarios, which will

be defined in the Formulation of Scenarios Report of the Safety Case Portfolio. Variant scenarios include, for example, the presence of one or more defective canisters, and the possibility that the buffer and/or backfill do not reach their respective target states due to misplacement or early piping and erosion (which could arise, for example, if rock suitability criteria - RSC - are not strictly followed), thus compromising the protection they afford to the canisters. The buffer and/or backfill could also potentially be degraded in the relatively short term (i.e. prior to major climate change) by e.g. bentonite-cement or bentonite-iron interactions.

Unlikely FEPs that could compromise the containment safety function of the canister are considered in disturbance scenarios. Disturbance scenarios include, for example, one or more canisters with a relatively large penetrating defect (≥ 1 mm), failure of one or more canisters by rock shear and significant loss of buffer by exposure to dilute (and probably oxygenated) glacial melt water, and/or high groundwater flow rates leading to corrosion failure of one or more canisters.

2.2 Types of analyses

Radionuclide transport modelling is used to quantify activity release rates to the surface environment, as well as transport through the surface environment. It is also used to explore sensitivity of the calculated results to uncertainties in, e.g. the location and numbers of failed canisters and in the transport and retention properties of the various media within which radionuclides subsequently migrate. In the 2012 safety case, radionuclide transport modelling will be applied in:

- probabilistic sensitivity analysis (Ch. 5);

and in the evaluation of deterministic calculation cases supporting the assessment of:

- dose (Ch. 6); and
- geo/bio fluxes (Ch. 7).

Probabilistic sensitivity analysis will be applied, in the first instance, to the parameters used to model the variant scenario in which one or more canisters with penetrating or near-penetrating defects are present in the repository. The defective canisters are equally likely to be present at any location in the repository that satisfies relevant RSC. Probabilistic sensitivity analyses of other scenarios will be carried out if time/resources permit and, based on the first analyses, this is judged useful. The purpose of these probabilistic sensitivity analyses is to identify the input parameters or combinations of input parameters (lumped parameters) that control the geo-bio radionuclide fluxes produced by the repository.

Deterministic calculation cases will be defined and analysed for a range of variant and disturbance scenarios that encompass all lines of evolution leading to radionuclide release over a million year time period.

2.3 Calculation cases

For the analysis of near-field release and transport and geosphere transport, a reference case will be defined, together with a number of sensitivity or “what-if” repository calculation cases that explore the impact of specific uncertainties, either individually or in combination. The sensitivity or “what-if” cases will, for the most part, take a more pessimistic view of uncertainties than the reference case. By comparing the results of a sensitivity or “what-if” case analysis with those of the reference case, the impact of specific uncertainties can be illustrated. Three classes of repository calculation cases can be distinguished:

- Sensitivity cases, which account for uncertainties in the knowledge of the state and behaviour of the system (or parts of it) in the long term, which is reflected in the variability of the data used in the analyses. Variant scenarios will be analysed by means of one reference case and a few sensitivity cases.
- “What-if” cases, which illustrate the impact of unlikely events and processes that could affect the repository during its evolution. The timing and magnitudes of the events and processes considered in the “what-if” cases are not necessarily regarded plausible in the present repository. Disturbance scenarios will be mostly analysed by “what-if?” cases.
- Other calculation cases, which aim to “check” the robustness of the system or part of the system against unexpected and sometimes hypothetical (causally unspecified) events and processes. “Other scenarios” will be analysed with these calculation cases.

A range of biosphere calculation cases will also be defined for dose assessment, based on assumptions of varying degrees of realism and conservatism. To evaluate compliance with regulatory dose criteria (Section 1.2), dose assessment need only be carried out in the period termed by Posiva the “biosphere assessment time window”. Furthermore, to avoid excessive conservatism in the outcome of the safety analysis, sensitivity cases that evaluate the impact of uncertainties in the repository system will be analysed only within the surface system base scenario and its reference case (deemed to be the most plausible). It is not yet decided whether “what-if?” cases, being more speculative or hypothetical in nature, will be coupled biosphere calculation cases. The surface system scenarios to be evaluated for the various types of near-field/geosphere calculations cases are shown in Table 2-1.

Table 2-1. Biosphere calculation cases to be evaluated for the various types of near-field/geosphere calculations cases.

Biosphere calculation cases	Near-field and geosphere calculation cases				
	Reference	Sensitivity		“What-if?”	Other
		Releases to surface environment within biosphere assessment time window	No releases to surface environment within biosphere assessment time window		
Reference	✓	✓	×	×	×
Sensitivity	✓	×	×	×	×
“what-if”	✓	×	×	×	×
“other”	×	×	×	×	×

3 GROUNDWATER FLOW MODELLING

3.1 Roles of groundwater flow modelling

Groundwater flow and radionuclide transport modelling provides the starting point in the analysis of the radiological consequences of any scenario leading to radionuclide releases during the time window for which dose assessment is to be carried out. Flowing groundwater is the principal medium by which radionuclides released from a failed canister can be transported to the surface environment. Groundwater flow modelling is needed to quantify groundwater flow rates at potential locations of failed canisters, the relevant properties of all transport pathways from the failed canister to the surface environment, and the discharge locations in the surface environment, as well of uncertainties in each of these quantities.

Although not discussed further in this report, groundwater flow modelling is also needed in the context of barrier performance assessment (scoping calculations) and in the formulation of scenarios. In particular, it is used to assess the impact of hydraulic loads (i.e. relatively high groundwater flows around deposition holes and tunnels) on the repository barriers. Such flows may, for example, convey dilute or oxygen-bearing glacial melt water to repository depth, leading to buffer erosion and/or canister corrosion. Groundwater flow modelling can support the identification of unfavourable locations within the repository with respect to such processes, as well as estimates of the probability of significant detriment to the safety functions of the barriers at such locations: a relatively high probability of significant detriment indicates that the process can give rise to variant scenarios; a small but non-zero probability of significant detriment is a feature of disturbance scenarios.

3.2 Modelling approaches

Groundwater flow is currently modelled using both equivalent porous medium (EPM) and discrete fracture network (DFN) approaches, using the codes FEFTRA and ConnectFlow, respectively. These two codes are described later in this chapter. The EPM and DFN approaches each have their own advantages and limitations. DFN modelling includes a statistical description of the fracture distribution in the bedrock on a detailed scale. However, practical limitations of the DFN modelling carried out so far are that the density dependence of flow is not taken into account and that only steady state flow conditions have been simulated in different statistical realisations of the fracture network. EPM modelling includes deformation zones as discrete features, but otherwise applies average properties to the rock volumes between these features. It can, however, deal with transient conditions, and EPM flow simulations have thus been used to address the evolving flow conditions in the repository near field and at the site scale during repository operation and in the post-closure period.

In the 2012 safety case, DFN modelling will be applied for simulation of transport and retention along the release paths at the scale of the individual deposition holes. DFN modelling is well suited for assessment of the retention and detailed scale flow properties, because both are largely determined by the fracturing and fracture properties. Steady state simulations will be carried out for a few representative times after closure

of the repository. In this respect, the general approach to the simulations is similar to that used in the previous RNT-2008 analysis. However, the repository tunnels and EDZ will be included to the DFN flow model.

EPM modelling will be applied to assess evolution of the site scale flow conditions in different scenarios. EPM modelling is able to address flow related processes such as density dependent flow and transport of salt, flow driven by the temperature differences and heat transfer, transient flow and evolving boundary conditions.

Assessment of the degree of consistency between DFN and EPM approaches is one of the reasons to apply both models to evaluate the near-field flow rates. Another reason is that the effective scale of the near-field flow rates varies significantly. The flow rates around a deposition hole can be controlled by the flow properties of individual fractures and therefore require a DFN description. On the other hand, the flow rates along the disposal tunnels are controlled by repository scale flow conditions and possibly influenced by saline water, which calls for site scale EPM modelling.

3.3 ConnectFlow

ConnectFlow is a suite of computational tools for modelling groundwater flow and transport in both fractured and porous media on a variety of scales. It has been developed by Serco Assurance (formally AEA Technology, UK) over the last 10 years under a quality system that conforms to the international standards ISO 9001 and TickIT.

ConnectFlow includes the NAMMU equivalent porous medium (EPM¹) module and the NAPSAC discrete fracture network (DFN) module². ConnectFlow is also the name given to the concept of nesting NAMMU and NAPSAC sub-models into a combined EPM/DFN model. Using this concept, local DFN models that represent the detailed flow in fractures around tunnels, shafts, canisters or boreholes can be nested within a EPM model that extends the model to appropriate boundaries.

ConnectFlow can model steady-state and transient constant-density groundwater flow. Advective transport through a combined DFN/EPM is simulated by a particle tracking based approach. ConnectFlow supports the calculation of the flow-dependent solute retention property, the F -factor, along the flow paths. The F -factor is equivalent to the transport resistance WL/Q applied in the Posiva's modelling ($F = 2WL/Q$). W is the width of the transport path along which advection occurs, L is the transport distance and Q is the flow rate through the path. ConnectFlow particle tracking result files for the flow paths are directly applicable for the radionuclide migration analysis using the MARFA code (Section 4.3).

¹ The term *continuous porous medium* (CPM) is also sometimes used. CPM and EPM are usually used as synonyms. However, a distinction is sometimes drawn regarding the treatment of discrete elements. In both types of model, hydraulic properties are represented by equivalent values. An EPM model may, however, include e.g. HZs represented by 2D elements and background rock by 3D elements. A CPM model is more strictly continuous model, so that, e.g. in CONNECTFLOW's NAMMU, there are only 3D elements and transmissivities of the HZs are taken into account in the conductivity of the elements that are intersected by the HZs.

² <http://www.connectflow.com/>

ConnectFlow has been applied in the previous RNT-2008 radionuclide transport analysis for the assessment of the potential release paths from the repository and calculation of the transport resistance WL/Q for potential radionuclide release paths from the repository.

In the 2012 safety case, ConnectFlow will be used to analyse retention properties along the potential release paths from the repository and to assess the groundwater flow rates around the deposition holes. ConnectFlow is able to provide spatial coupling between the radionuclide source location in the repository and corresponding discharge location to the biosphere.

3.4 FEFTRA

FEFTRA is a finite element program package developed at VTT, Finland, for groundwater flow analyses in Posiva's site evaluation programmes. The code is capable of modelling steady-state or transient groundwater flow, solute transport and heat transfer as coupled or separate phenomena. The mathematical model consists of partial differential equations written for hydraulic head/pressure, solute concentration and temperature. The equations are coupled by means of the Darcy velocity as well as temperature and concentration dependent properties such as fluid density. When simulating solute transport, the effect of matrix diffusion can be taken into account, and highly convective cases can be handled with different upwind methods. The time discretisation in FEFTRA is based on the finite difference approximation. The matrix equations resulting from the finite element formulation can be solved either using the direct frontal solver or various iterative solvers. In coupled cases, a set of nonlinear algebraic equations is solved applying the Picard iterative approach with options for the relaxation.

The FEFTRA code allows the use of linear or quadratic one-, two- and three-dimensional elements. In three-dimensional groundwater flow simulations, sparsely fractured rock can be described by three-dimensional elements, fracture zones or other planar structures by two-dimensional elements and tunnels by one-dimensional elements. The finite element mesh is refined around natural and engineered bedrock structures (e.g. fracture zones, sinks, tunnels, etc.) (static mode) or at the locations with high hydraulic gradient (dynamic mode) by a quadtree/octree algorithm.

FEFTRA has been applied in the previous safety analyses to analyse evolution of the density dependent flow conditions after the closure of the repository taking into account also the heat generated by the waste. The model includes underground tunnels and it has been calibrated to various in-situ hydraulic tests and hydraulic effects of the ONKALO tunnel. Groundwater flow rates in the previous performance assessment along the repository tunnels and in the repository have been based on the FEFTRA simulations.

As described in later chapters, FEFTRA will be used in conjunction with ConnectFlow to simulate groundwater flow conditions around and in the repository for the different scenarios of the 2012 safety case.

4 RADIONUCLIDE RELEASE AND TRANSPORT MODELLING

4.1 Radionuclide release and transport processes

In most of the calculation cases that will be considered in the 2012 safety case, radionuclides released from a failed canister will be dissolved in water and conveyed in solution through the repository near field and through the geosphere towards the biosphere or surface system (the issues of gas- and colloid-mediated transport will, however, also be considered in some calculation cases). The most important radionuclide transport and retention processes, which are included in near-field and geosphere transport models, are advection, diffusion and sorption. These are described briefly in the following paragraphs, together with a short description of release processes.

Radionuclide release from a failed canister

Following canister failure and contact of the fuel with water, there will be a relatively rapid release to solution of the radionuclide inventory at grain boundaries and in gaps. This part of the radionuclide inventory is termed the instant release fraction, or IRF, since its release to solution is conservatively modelled as instantaneous. Release of the IRF will be followed by a slower, congruent release of radionuclides from the fuel matrix, the cladding and other metal components. It is assumed in safety assessment modelling that the inventory of activation products in Zircaloy and other metal parts is released congruently with the corrosion of the metal. The slow, long-term release of radionuclides from the fuel matrix is handled in safety assessment modelling by assuming a constant fuel degradation rate, leading to constant release rates of radionuclides from the matrix.

Radionuclides will either enter solution, form volatile species that can mix with repository-generated gas (relevant for C-14), or, if their solubilities in water are low, precipitate either as immobile solids or as colloids. They may also sorb onto solid surfaces, such as those of the iron oxyhydroxides formed by corrosion of the iron insert of the canister, but this process is conservatively omitted in modelling. Dissolved radionuclides and radionuclides in gaseous form are modelled as uniformly distributed in the void space in the canister interior, from where they migrate into the surrounding buffer, and from there into the geosphere. If the canister fails due to the presence of a small hole (e.g. a penetrating defect in the weld), the transport resistance provided by this hole significantly limits the transport of solutes, and can be taken into account in modelling release rates from the canister. The transport resistance of the hole will vary over time. It will increase if the hole becomes clogged with bentonite and/or corrosion products. It may be reduced, e.g. if the corrosion of the insert leads to larger-scale rupturing of the copper. The effects of these different possibilities will be explored in sensitivity analyses.

Advection, dispersion and diffusion

If the buffer performs in accordance with its performance targets, the dominant radionuclide transport process through the buffer will be diffusion. Any colloids formed

if solubility limits are exceeded are assumed to be immobile in the buffer. In a KBS-3V repository, radionuclides may diffuse from the buffer to the geosphere by three alternative paths, characterised by three effective flow rates, Q_F , Q_{DZ} and Q_{TDZ} , respectively (Fig. 4-1):

- from the buffer directly to a host rock fracture intersecting a deposition hole (Q_F);
- from the buffer to the deposition tunnel EDZ (Q_{DZ}); and
- from the buffer to the deposition tunnel backfill and thence to a fracture intersecting the deposition tunnel (Q_{TDZ}).

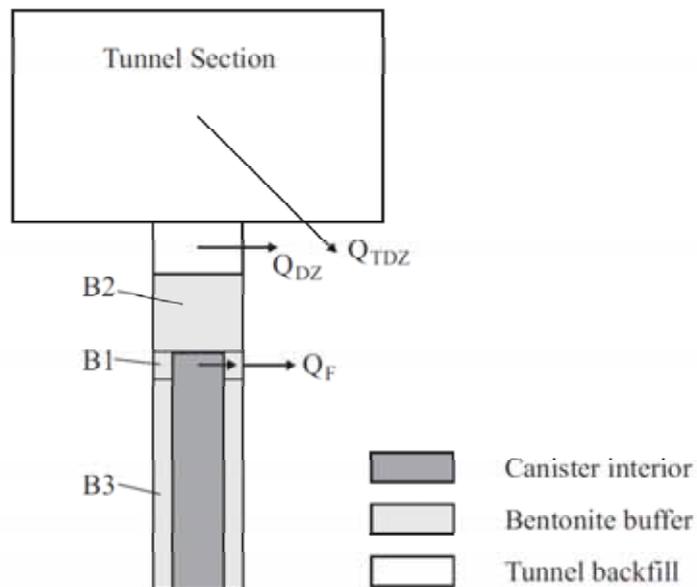


Figure 4-1. The near-field model for a KBS-3V repository to be calculated using GoldSim.

The main transport processes in the geosphere are illustrated in Figure 4-2. Radionuclides will be transported through transmissive fractures that exist throughout the host rock predominantly by advection, i.e. by the bulk motion of flowing groundwater. These fractures form a connected network that could ultimately lead to released radionuclides being conveyed to the biosphere. The geosphere transport resistance, denoted as WL/Q , is the main hydrogeological parameter characterising advection along an individual transport path through the network. Variations in the flow field within individual fractures coupled with mechanical mixing and molecular diffusion can result in local water flows and velocities that differ from the larger-scale average, resulting in the spreading of radionuclide releases in a process termed hydrodynamic dispersion.

In fracture planes and in the wall rock adjacent to them, there are numerous water-filled void spaces and rock matrix pores where water is effectively stagnant. Here, diffusion of solutes in the rock matrix (matrix diffusion) coupled to sorption on matrix pore surfaces is the dominant retention mechanism in the geosphere for many radionuclides. Even for non-sorbing species, matrix diffusion may provide an efficient temporal

retardation and spreading of the releases simply by removing these species from the flowing groundwater.

Previous Posiva's safety analyses have represented properties of generic rock matrix along the flow paths by two different layers (see, e.g. Nykyri et al. 2008b and Fig. 4-2): the first centimetre in contact with the fracture and the next 9 cm deeper in the granite. The 1cm layer closest to the fracture is assigned a significantly higher porosity and diffusivity with respect to the bulk of the rock matrix. This increased porosity and diffusivity may be due, e.g. to mineralogical alteration. Diffusion is possible in this layer and in a 9 cm unaltered layer adjacent to it. The rock matrix beyond these two layers is conservatively assumed to be inaccessible to diffusion. Ongoing geological site investigations aim to establish site-specific models of rock matrix structure and retention process. So far, four different retention models have been tentatively identified. The number of rock matrix layers in these models varies between one and three different layers.

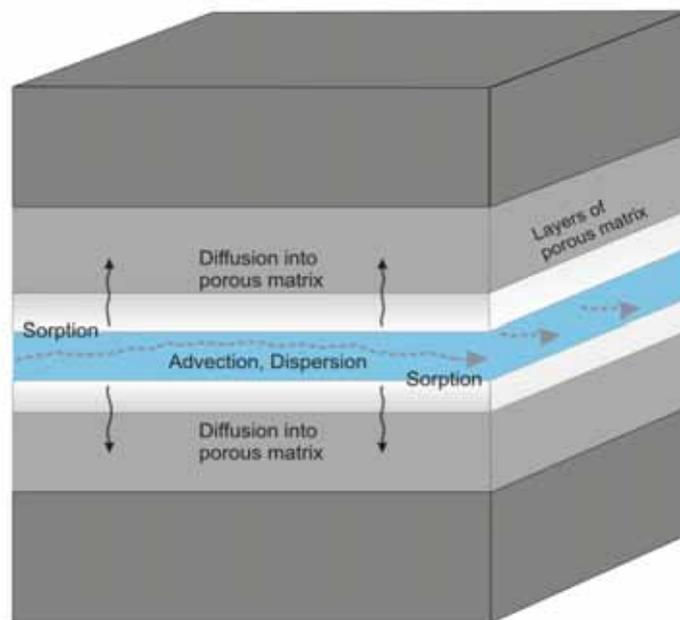


Figure 4-2. *The main transport processes in the geosphere. In flow and transport models, diffusion-accessible pore space may be assumed to exist throughout the rock matrix, or to be confined to spatially limited zones adjacent to transmissive fractures.*

Sorption

Sorption is a general term describing the attachment of dissolved species to mineral surfaces. It includes ion exchange, physical adsorption and surface complexation. Sorption is element specific and depends on both the aqueous speciation of radionuclides, and the solid phase composition and surface characteristics.

In transport modelling, the sorption of radionuclides on the pore surfaces of the buffer and rock are taken into account. Equilibrium sorption is assumed (i.e. kinetics are fast compared with transport processes), such that the degree of sorption may be quantified by a species-dependent distribution coefficient (K_d). K_d is strongly dependent on the prevailing chemical conditions, so its value may change, e.g. if the redox conditions or temperature changes, if the sorbing solid surfaces dissolve or if they undergo other mineralogical transformations.

4.2 GoldSim and its contaminant transport module

General description

GoldSim is a Monte Carlo simulation software solution for dynamically modelling complex systems in business, engineering and science.³ It has a specialised contaminant transport module (GoldSim RT), allowing application of GoldSim in radioactive waste management.

The contaminant transport module allows the user to explicitly represent the following processes:

- Release of mass (e.g., radionuclides) from specified sources, taking into account both canister failure and the degradation of any materials in which the contaminants are bound (e.g., spent fuel).
- Transport of contaminants through multiple transport pathways within an environmental system (e.g., the repository near field or geosphere). The transport pathways can consist of multiple transport and storage media (e.g., groundwater, buffer, backfill, rock), and both advective and diffusive transport mechanisms can be directly simulated. Transport modelling along the pathways includes solubility constraints and partitioning of contaminants between the media present in the system, and can handle multiple radioactive decay chains of unlimited length.

GoldSim can also handle biological transport pathways, although it is not planned to use this facility in the 2012 safety analysis.

The fundamental outputs produced by GoldSim RT are mass fluxes at specified locations within the system, and concentrations within the transport and storage media.

In previous Posiva safety analyses, the radionuclide transport from the repository to biosphere has mostly been computed with the near-field release and transport code REPCOM and the geosphere transport code FTRANS. However, for the 2012 safety assessment, REPCOM will be superseded by GoldSim for all near-field release and transport calculations. Geosphere transport calculations will also be carried out using either GoldSim or the code MARFA (Section 4.3).

³ www.goldsim.com

There are several reasons for replacing REPCOM with GoldSim. Firstly, GoldSim RT allows modelling that is more realistic in some respects compared with REPCOM. In particular, unlike in REPCOM, solubility limits can be imposed throughout the buffer and in the backfill, and isotopes of the same element are properly coupled in multiple decay chains. GoldSim is also well suited for use in the probabilistic sensitivity analyses planned for the 2012 safety case (Ch. 5), including, for example, post-processing tools to perform statistical analyses on the results of multiple realisations. Furthermore, from the point of view of managing the analysis of calculation cases, there are clear benefits of using a single code for (at least some) integrated near-field and geosphere calculations. Finally, the user interface of GoldSim is easier, more user-friendly, more illustrative and clearer than that of REPCOM.

The applicability of GoldSim to relevant problems has been tested in code verification exercises using REPCOM and FTRANS (see code verification report).

Input parameters specifying isotopes and decays

Listings of isotopes and decays must be provided for near-field release and transport modelling and for geosphere transport modelling. The input parameters comprise:

- isotope name (e.g. I-129);
- half life (in years); and
- names of daughters (if any).

Input parameters for near-field release and transport modelling

The main physical and chemical input parameters for near-field release and transport modelling with GoldSim may be grouped as follows:

- inventories;
- chemical and transport properties;
- diffusion areas;
- other data.

Data in the group *inventories* comprises, for each isotope considered:

- uranium inventory per canister (in tonnes);
- inventory (GBq/tU);
- partitioning between fuel matrix, IRF, Zircaloy and other metal parts (in %ages) and the amounts of stable isotopes in each group.

Data in the group *chemical and transport properties* comprises, for each isotope (or chemical species) considered:

- near-field solubility limit (in moles per litre);

and for each isotope and each component where transport and retention are modelled

(the buffer and the deposition tunnel backfill⁴):

- sorption coefficient (K_d in $\text{m}^3 \text{kg}^{-1}$);
- porosity;
- effective diffusion coefficient (D_e in $\text{m}^2 \text{s}^{-1}$);

Data in the group *diffusion areas* comprises, for each boundary between components, and for a set of consecutive time windows (if needed):

- the area across which transport takes place.

Data in the group *other data* comprises:

- grain density of the buffer material (in kg m^{-3});
- grain density of the buffer material (in kg m^{-3});
- degradation rate of the fuel matrix (in a^{-1});
- degradation rate of zircaloy (in a^{-1});
- degradation rate of other metal parts (in a^{-1});
- void volume in the canister interior (in m^3);
- three effective flow rate, Q_F , Q_{DZ} and Q_{TDZ} (in $\text{m}^3 \text{a}^{-1}$), which describe the rate of transfer from the near field to the geosphere (see Fig. 4-1; note that, in the case of a KBS-3H repository, only the effective flow rate Q_F is relevant);
- the vertical thickness of the deposition tunnel EDZ where this intersects a deposition hole (needed to calculate the area across which radionuclides are released to the EDZ from the buffer).

The effective flow rates will be determined from the results of EPM modelling using FEFTRA and DFN modelling using ConnectFlow. It should be noted, however, that, for steady state flow conditions, the EPM and DFN simulations should show consistent results regarding the both the flow rates around the repository and the characteristics of flow and potential radionuclide transport paths at the site scale. The interface between ConnectFlow and the GoldSim near-field model is described in detail in Section 5-5.

Input parameters for geosphere transport modelling

The main physical and chemical input parameters for geosphere transport modelling with GoldSim may be grouped as follows:

- fracture transport and retention properties;
- rock matrix geometry;
- rock matrix transport and retention properties.

Data in the group *fracture transport and retention properties* comprises:

- the transport resistance WL/Q (in a m^{-1});
- longitudinal dispersion coefficient (in $\text{m}^2 \text{s}^{-1}$);
- the sorption coefficient for the surface sorption on fracture surfaces (in m^{-1}).

⁴ The near-field model does not explicitly include transport through the deposition tunnel EDZ.

Data in the group *rock matrix geometry* comprises:

- the number of rock matrix layers (generally either one or two);
- the thickness of each rock matrix layer (in m).

Data in the group *rock matrix transport and retention properties* comprises, for each isotope (or chemical species) considered and for each rock matrix layer:

- sorption coefficient (K_d in $\text{m}^3 \text{kg}^{-1}$);
- porosity (ε);
- effective diffusion coefficient (D_e in $\text{m}^2 \text{s}^{-1}$);

WL/Q , which is the main hydrogeological input parameter of the GoldSim geosphere transport model, will be determined principally by DFN flow modelling carried out with ConnectFlow in conjunction with particle tracking. WL/Q is not a single-valued property of the rock. Rather, it is a characteristic of each transport path, and may vary significantly between paths, depending, for example, on where in the repository a given transport path originates. Furthermore, each DFN realisation of the stochastic fractures in the rock will give rise to a somewhat different distribution of WL/Q . Thus, for the purposes of GoldSim geosphere transport modelling, the ConnectFlow output that is of interest is the distribution of WL/Q for each repository panel from multiple DFN realisations (Fig. 4-3).

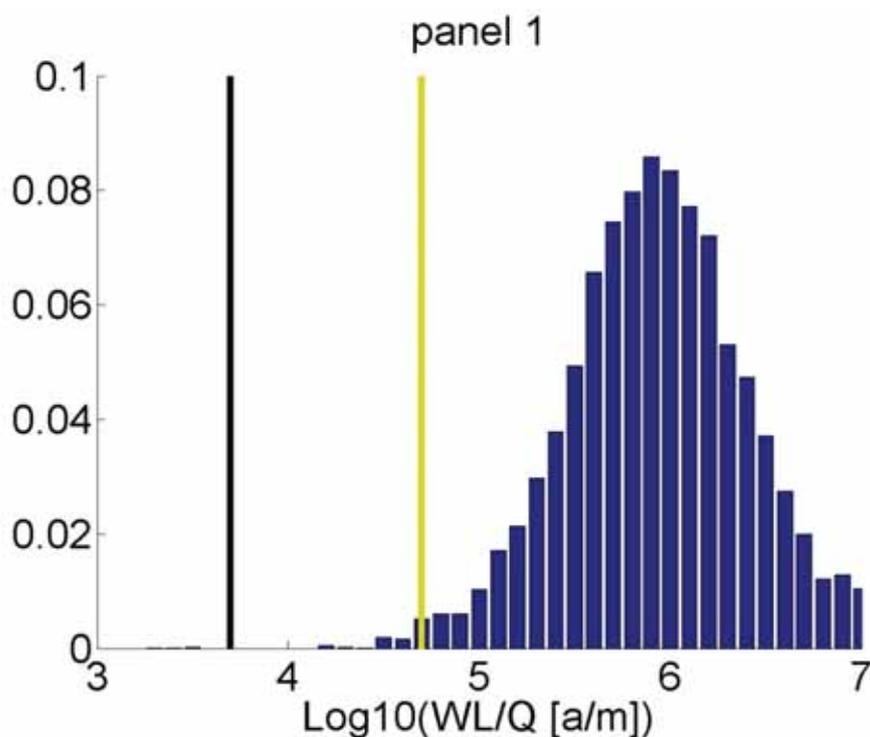


Figure 4-3. The distribution of $\log_{10}(WL/Q [a/m])$ in 21 DFN realisations from panel 1 of a KBS-3V repository at 1 000 years (after Fig. 4-18 of Nykyri et al. 2008). The vertical bars show the proportion of canister positions with WL/Q values in a given interval.

The interface between ConnectFlow and the GoldSim near-field model is also described in detail in Section 5-5.

4.3 MARFA

General description

The computer code Migration Analysis of Radionuclides in the Far Field (MARFA) uses a particle-based Monte Carlo method to simulate the transport of radionuclides in a sparsely fractured geological medium (Painter & Mancillas 2009). The physical processes represented in MARFA include advection, longitudinal dispersion, Fickian diffusion into an infinite or finite rock matrix, equilibrium sorption, decay, and in-growth. Multiple non-branching decay chains of arbitrary length are supported.

MARFA can accept pathway trajectories from the discrete fracture network groundwater flow code ConnectFlow (Section 3.3). The pathway trajectories represent the movement of hypothetical, advectively transported groundwater tracers along pathways from radionuclide source locations. MARFA then solves radionuclide transport along the pathways using a time-domain particle method. With this method, particles are advanced along a pathway using deterministic spatial displacements and random transit times for each step. MARFA supports an arbitrary number of trajectories and source locations, full spatial variability for all pathway properties, and full temporal variability in radionuclide source strength. It can also represent radionuclide transport in a time-dependent flow field arising, e.g. from glacial rebound and changing climate states in the future. The Monte Carlo algorithm in MARFA produces output in the form of particle arrival times at pathway end points. Cumulative mass discharge (cumulative breakthrough) at a given time can be constructed from the arrival times.

Present versions of MARFA are able to handle matrix diffusion in only a single layer of the rock matrix. MARFA will be updated to allow inclusion of the new site-specific multi-layer matrix retention models, as described in Section 4.1, during 2010.

Input parameters for geosphere transport modelling

The main physical and chemical input parameters for geosphere transport modelling with MARFA may be grouped as follows:

- elements, isotopes and decays;
- near-field source term;
- rock matrix retention properties;
- flow path properties

Data in the group *elements, isotopes and decay* comprises:

- element names;
- isotope names;
- decay constants (in a^{-1});

- description of the decay chains (structure of the decay chains is embedded to the input format).

Data in group *near field source term* comprises:

- source names;
- range trajectories for each source;
- unit of the source (in Mol a⁻¹ or Bq a⁻¹);
- time series of source terms for different isotopes;
- time [a], source for each isotope (in Mol a⁻¹ or Bq a⁻¹).

If multiple flow periods are modelled, then possible effects of the flow changes to the source term need to be presented consistently in the time series of the source compared to the parameter data on the flow changes in the *rock matrix retention properties* and *flow path properties* data groups.

Data in group *rock matrix retention properties* comprises⁵:

- name of the rock type, and for each rock type;
- longitudinal dispersion coefficient (in m² s⁻¹);
- for each element, the parameters (i), κ , as defined below, (ii), Δ/D_e , where Δ is the thickness of the matrix (in m) and D_e (in m² a⁻¹) is the effective diffusion coefficient of the matrix, and (iv), K_a , the sorption coefficient for the surface sorption on fracture surfaces (in 1/m).

In the above:

$$\kappa = \sqrt{\varepsilon D_e R},$$

where ε is matrix porosity and R is the retardation coefficient for the matrix.

If different flow periods are defined, then above information need to presented for each flow period. If multiple layers of the rock matrix are modelled, then above information is needed for each layer of the rock matrix;

Data in group *flow path properties* comprises:

- ConnectFlow trajectory information for different segments of the flow paths including, (i), end coordinates of the segments along the path, (ii), name of the rock type for the segment, (iii), advective travel time over the segment (in a) and (iv), the F-factor $F = 2WL/Q$ (in a m⁻¹).

⁵MARFA will be updated so that it is able handle multiple layers of rock matrix. Input data for that option is not yet defined. The text above gives data mainly for a single limited layer of rock matrix, but it should also be broadly applicable to the multi-layer case

4.4 Surface system models and codes

As noted in Chapter 1, the scope of the present document includes radionuclide transport modelling in the repository system and at the interface between the repository system and the surface system. Radionuclide transport processes in the various ecosystems in the biosphere are outside the scope, but the models used are described briefly here, since the handling of the interfaces with these models is discussed in this document.

Groundwater flow, water table characteristics and radionuclide transport at the interface between the repository system and the surface system are handled by the surface and near-surface hydrological model (SNSHM), documented in Karvonen (2008, 2009a,b). The SNSHM is a 3-dimensional model in which the overburden and the bedrock are combined in single numerical solution of flow and transport. The model links unsaturated and saturated soil water in the overburden and groundwater in bedrock into one continuous system, characterised by a pressure distribution. Horizontal and vertical water fluxes can be obtained as output values. For radionuclide transport modelling, radionuclides in the overburden may be treated as inert particles that “go with the flow”, or K_d -values may be assigned to them (if values can be justified).

Input to the SNSHM comes from terrain and ecosystem development modelling (TESM). The future terrain and ecosystems are forecast with a geographical information system (GIS) toolbox called UNTAMO (Ikonen et al. 2010). Briefly, the toolbox consists of the following main components:

- land uplift and delineation of the sea area;
- surface water bodies;
- terrestrial and aquatic erosion;
- accumulation of organic matter;
- terrestrial vegetation;
- aquatic vegetation;
- faunal habitats;
- human settlement and land use; and
- simulation control.

For radionuclide transport modelling using the SNSHM, further input comes from the distribution and evolution of radionuclide releases from the geosphere computed using MARFA.

The SNSHM provides the groundwater head boundary conditions for deep groundwater flow modeling. Furthermore, both TESHM and the SNSHM provide input for setting up the landscape model (LSM), which is a time-dependent and site-specific model used to simulate radionuclide transport through the various ecosystems of the biosphere, implemented using the code Pandora (Astrand et al. 2005). TESHM delineates a set of biosphere objects, each of which represents a sub-area within the modelled biosphere that can potentially, directly or indirectly, receive radionuclides released from the repository. Each biosphere object is described by one, or more, ecosystem types. The spatial and temporal distribution of possible radionuclide release paths to the biosphere objects is provided by SNSHM. The LSM, in turn, provides input to radiological consequences analysis.

5 PROBABILISTIC SENSITIVITY ANALYSES

5.1 Aims of the analyses

In safety assessment, it is of interest to know to which parameters, or combinations of parameters (lumped parameters), the results of model calculations are most sensitive; i.e. the extent to which the variance in model output is affected by variance in various uncertain inputs, expressed as probability density functions (PDFs). This provides both feedback to the RTD programme (where would uncertainty reduction be most beneficial) and also can reduce the number of (deterministic) calculation cases that need to be defined for consequence analysis. Sensitivity analysis using probabilistic techniques (Monte-Carlo simulation) provides a useful tool to these ends.

5.2 Model chain

The model chain for probabilistic sensitivity analyses is illustrated in Fig. 5-1. As noted in Section 4.2, GoldSim is well suited for use in the probabilistic sensitivity analyses (PSA) planned for the 2012 safety case, and it is thus planned to use GoldSim for both near-field release and transport and for geosphere transport modelling in the PSA. The end-point of the GoldSim calculations will be activity release rates to the biosphere (geo-bio fluxes). Flow modelling to support the selection of groundwater-flow-related parameters used in GoldSim model will be carried out with ConnectFlow. No biosphere (landscape) modelling is planned for these sensitivity analyses, and the pattern of radionuclide releases to the biosphere does not need to be considered.

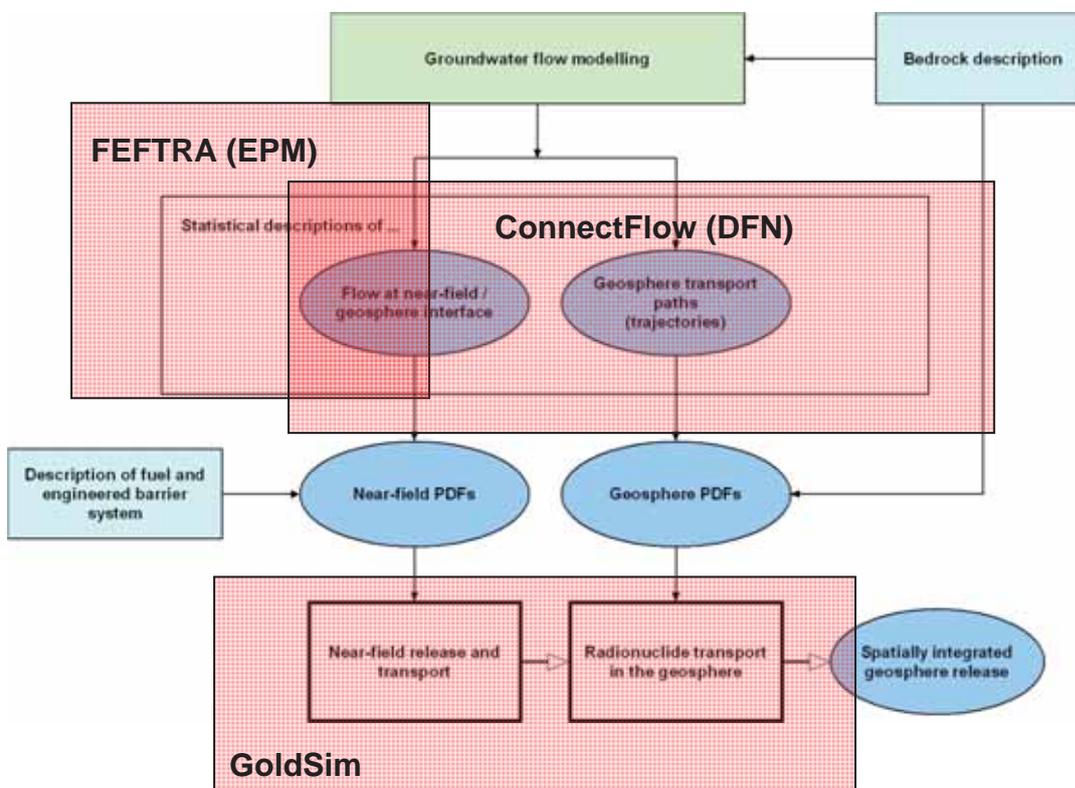


Figure 5-1. Model chain for probabilistic sensitivity analyses.

5.3 Flow modelling

Using ConnectFlow, local DFN models that represent the detailed flow in fractures around tunnels, shafts, canisters or boreholes can be nested within an EPM model that extends the model to appropriate boundaries (Section 3.3). Multiple DFN realisations will be created in order to explore the effects of uncertainty in the the spatial distribution of non-deterministic water conducting features in the site.

The DFN realisations will include all canister locations and flow rates along the fractures intersecting the repository deposition holes, such that Q_F can readily be calculated. In addition, the DFN modelling will also provide information on the length of the fracture on the wall of the deposition hole if needed (angle of the intersection between the deposition hole and fracture). The deposition tunnel EDZ will be included to the model as a planar structure with constant transmissivity and thickness below the repository tunnels. The flow rate along this structure is known at the location of each deposition hole (Q_{DZ}). The tunnels themselves are included in the DFN flow model as an EPM submodel. Therefore, flow rates along the tunnels are also known (Q_{TDZ}).

In previous Posiva safety analyses, the deposition holes containing failed canisters have been coupled to the length of deposition tunnel that corresponds to each hole (tunnel section) and it has been assumed that the geosphere release path starts from these sections of the tunnels, i.e. each tunnel section is intersected by a fracture. When the whole repository and all canister locations are simulated in the same model, as is planned for the 2012 safety case, it is quite probable that the release pathways from different canisters to the tunnel may end up to the same fracture intersecting the tunnel. This means that length of the flow path along the tunnel and flow rate in the tunnel can vary between different canister locations. This complicates the interfacing between GoldSim and groundwater flow modelling (Section 5.5). Note, however, that previous safety analyses have concluded that in the overall performance of the repository system the release pathway via the tunnel is insignificant.

Selection of the suitable starting locations for the transport paths in the simulations needs to fulfil the Rock Suitability Criteria (RSC) that will be applied in the actual process of the final disposal. In practice, this requires that ConnectFlow simulations need to be repeated both for the open repository and for the post closure conditions. More specifically, the following steps are to be carried out to analyse the ranges of possible retention properties along potential radionuclide transport paths from the repository and to assess the possible ranges of groundwater flow rates around the deposition holes:

1. Perform groundwater flow calculations with multiple DFN realisations of stochastic water-conducting features. For each realisation, calculate early (pre-saturation) flow and long-term flow.
2. Use open repository flow results to identify - for a given DFN realisation - which canister positions satisfy the RSC (inflow criteria).
3. For each DFN realisation, use particle tracking to identify/characterise long-term transport pathways from each canister location in terms of WL/Q . Filter results to exclude locations not satisfying the RSC.

4. From the multiple DFN realisations, develop ensemble of pathways from each canister location (distribution of characteristics arising from both spatial heterogeneity and uncertainty associated with the spatial distribution of non-deterministic water-conducting features).
5. For each DFN realisation, calculate the near-field flow rates Q_F , Q_{DZ} and Q_{TDZ} for each canister location⁶. Filter results to exclude locations not satisfying the RSC.

5.4 Radionuclide release and transport modelling

Probabilistic sensitivity analysis will be applied, in the first instance, to the variant scenario in which one or more canisters with initial penetrating or near-penetrating defects are present in the repository. Each individual GoldSim simulation will sample the necessary input parameters defined PDFs (e.g. buffer and rock matrix retention parameters), as well as a set of flow-related parameters for a randomly selected transport pathway from the ensemble of pathways calculated by flow modelling (see Section 5.5 for further details). Fig. 5-2 illustrates the sampling of the flow-related parameter WL/Q , as it was done in preliminary probabilistic calculations. For the 2012 safety case a different approach is intended: WL/Q will be sampled from a table generated with ConnectFlow described in section 5.5 (instead of from a PDF).

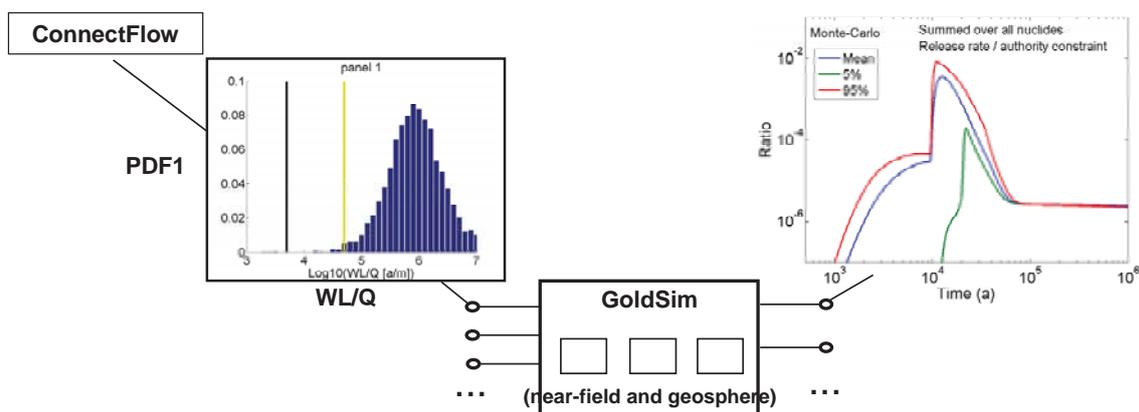


Figure 5-2. Sampling a distribution of WL/Q for probabilistic sensitivity analysis.

GoldSim will represent the multiple transport paths from a failed canister location to the biosphere by three representative transport paths, one for near-field releases via a fracture (F), one for releases via the tunnel disturbed zone (DZ) and one for releases via the tunnel backfill (TDZ), each characterised by a sampled transport resistance, WL/Q . Note that these may well vary markedly (e.g. if the tunnel EDZ provides a “fast path” to a relatively transmissive fracture). The GoldSim model and its flow-related input are illustrated in Fig. 5-3.

⁶The results for Q_F and Q_{TDZ} will also be used for assessing the impact of hydraulic loads on the repository barriers (i.e. the assessment of processes such as the possible infiltration of dilute or oxygen-bearing glacial meltwater to repository depth).

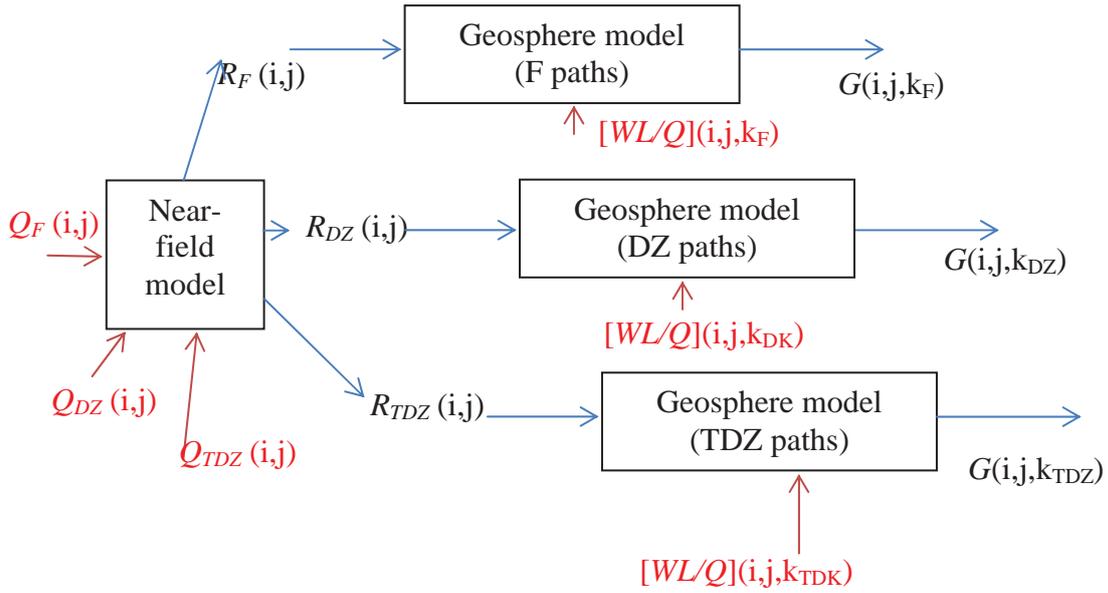


Figure 5-3. The GoldSim near-field release and transport and geosphere transport model for probabilistic sensitivity analysis. Flow-related input data for a single GoldSim realisation are shown in red.

The figure shows, as flow-related inputs, the near-field flows Q_F , Q_{DZ} and Q_{TDZ} for DFN realisation i and for deposition hole j . The corresponding near-field releases calculated by GoldSim are denoted as R_F , R_{DZ} and R_{TDZ} . It also shows the geosphere transport resistances for each of the corresponding geosphere transport paths.

For a given DFN realisation i and deposition hole j , ConnectFlow will provide unique values for Q_F , Q_{DZ} and Q_{TDZ} . Furthermore, ConnectFlow will provide several values for the transport resistance of the geosphere pathway that starts in the fracture that intersects the deposition hole ($[WL/Q](i,j,k_F)$, with $k_F = 1, \dots, v$) due to the heterogeneity of the granite formation. Similarly, the transport resistance through the geosphere pathways starting in the tunnel EDZ takes several values ($[WL/Q](i,j,k_{DZ})$, with $k_{DZ} = 1, \dots, w$). The same applies to the pathways starting in the deposition tunnel ($[WL/Q](i,j,k_{TDZ})$, with $k_{TDZ} = 1, \dots, x$).

In the probabilistic calculations (used in the PSA), in each individual realisations the overall activity release rate to the biosphere, $G(i,j,k)$, for realisation i , deposition hole j and one set of geosphere pathways ($k=k_F, k_{DZ}, k_{TDZ}$), is obtained by summing the 3 individual path releases shown in Fig. 5-3:

$$:G(i,j,k) = G(i,j,k_F) + G(i,j,k_{DZ}) + G(i,j,k_{TDZ}). \quad (5-1)$$

In the probabilistic sensitivity analyses, the ranges of the parameters considered reflect the full uncertainty and variability of the parameters, and not just the uncertainty associated with a best estimate value. The results of the sensitivity analyses should reveal, for example, which of the transport paths are most significant in determining the magnitudes of releases (i.e. do all paths contribute significantly, or only the fastest paths?).

5.5 Data flows and interfaces

The model interfaces that must be considered in the probabilistic sensitivity analyses are those between:

- near-field groundwater flow modelling using ConnectFlow and the GoldSim near-field release and transport model;
- far-field groundwater flow modelling using ConnectFlow and the GoldSim geosphere transport model; and
- the GoldSim near-field release and transport model and the GoldSim geosphere transport model.

Concerning the third interface, near-field release and transport modelling and geosphere transport will be carried out with a single integrated GoldSim model, whereby the activity releases to the geosphere will be made equal to the activity releases from the near-field.

The first two of these interfaces must be considered together, since the groundwater flow around the repository near-field (especially the flow Q_F) is expected to be inversely correlated with the geosphere transport resistance WL/Q , i.e. a more transmissive fracture intersecting a deposition hole is expected to give a relatively high value of Q_F and a low value of WL/Q .

A table of relevant ConnectFlow results will be developed to facilitate data transfer across the two ConnectFlow-GoldSim interfaces. The proposed form of the table is illustrated in Table 5-1. Each GoldSim simulation will sample randomly a set of three pathways (F, DZ and TDZ) for a given DFN realisation and deposition hole (e.g. the three grey rows in table 5.1). . The rows of the proposed table provide the following information:

- Column 1: A particle identification number for the particle tracks generated by ConnectFlow.
- Column 2: ConnectFlow DFN realisation number (i in Fig. 5-3).
- Column 3: Deposition hole number (j in Fig. 5-3).
- Column 4: Pathway type. F: particle exits deposition hole via an intersecting fracture; DZ: particle exits deposition hole and enters deposition tunnel EDZ; TDZ: particle exits deposition hole and enters deposition tunnel backfill.
- Column 5: The flow per unit width of fractures intersecting the deposition hole (Q/W). This column can be used to calculate the near-field flow Q_F by means of the equation:

$$Q_F = 2 \sqrt{8b_v D_w r_t \frac{Q}{W}}$$

where D_w is the diffusion coefficient of ions in free water, r_t is the deposition hole radius and b_v is the fracture aperture. The aperture may be

either assigned a fixed value, or be assumed to be proportional to the hydraulic aperture.

Note that, in earlier Posiva safety analyses, the quantity derived using the above equation was denoted Q_{bl} (boundary layer resistance). Q_F included the effects of this boundary layer resistance, and also the transport resistance of the buffer. The latter is now calculated explicitly by GoldSim. Note also that the above equation is valid only for calculation cases for a non-perturbed buffer-rock interface.

- Column 6: Not used by GoldSim. Rather, this information is used for assessing the possible erosion of the backfill. The fracture referred to here is the closest one to the deposition hole that intersects the deposition tunnel.
- Column 7: The values of Q/W in this column can be used to calculate the Q_{DZ} values required by the GoldSim near-field calculation. The easiest way to assess Q/W from the ConnectFlow model is use the local Darcy velocity. On 2D fractures the Darcy velocity equals Q/W . ConnectFlow model usually applies linear elements i.e. the Darcy velocity is constant over each element. If there are several elements along the intersection line, then either maximum Q/W (the main channel) or the average of this parameter may be used.
- Column 8: Q_{TDZ} calculated above a given deposition hole/canister location, to be used directly by GoldSim. Parameter will be non-zero if tunnels are included in the DFN model.
- Column 9: Length of transport path along tunnel to the nearest downstream fracture intersection (in the case that the tunnels are included in the DFN model). Can be used to set the length of the tunnel section modelled by GoldSim.
- Column 10: WL/Q value to be used directly by GoldSim.

Table 5-1. Table produced by ConnectFlow to be sampled by GoldSim.

Particle number	Realisation number [see note 1]	Deposition hole number	Pathway type	Near-field flows (Q/W)			Tunnel flow Q_{TDZ}	Tunnel path length	WL/Q for particle path
				for fractures intersecting deposition hole	for fracture intersecting deposition tunnel nearest the hole	for the DFN fracture representing the tunnel EDZ			
1	1	1	F	
2	1	1	F						
3	1	1	F						
4	1	1	DZ						
...	1	1...	DZ						
	1	1							
		..							
		..							
	1	1	TDZ						
N	1	1.	TDZ						
n+1	1	2	F						
n+2	1	2	F						
	1	2	DZ						
			..						

6 ANALYSES OF SCENARIOS REQUIRING DOSE ASSESSMENT

6.1 Aims of the analyses

Finnish regulations, as summarised in Section 1.2, imply that a dose assessment is required for those calculation cases in which radionuclide release to the biosphere occurs during a period referred to by Posiva as the biosphere assessment time window, extending at a minimum over several millennia. The calculations are needed to evaluate compliance with dose criteria, as well as to illustrate the impact of uncertainties on the calculated results.

Deterministic calculation for which dose assessments must be made again concern the reference case in the variant scenario in which one or more canisters with initial penetrating or near-penetrating defects are present in the repository. The unlikely, disturbance scenario in which a large earthquake leads to the failure of one or more canisters in the first few thousand years after emplacement may also lead to releases to the biosphere in this time window. However, the repository calculation cases defined to analyse the consequences of this scenario are likely to be classified as “what-if?” cases, and it remains to be decided whether these will be coupled any biosphere calculation cases for the assessment of dose (see Section 2.3).

6.2 Model chain

Somewhat different near-field/geosphere model chains will be used for calculations in which a dose assessment is to be made, compared with those for which it is not (Fig. 6-1). GoldSim will be used for all near-field release and transport calculations. GoldSim will also be used for geosphere transport calculations. However, to carry out a dose assessment, not only is the spatially integrated release rates of different radionuclides across the geo-bio interface as a function of time needed, but also the geographical distribution of the release locations. MARFA, used together with ConnectFlow modelling that includes the whole repository, is well suited to providing the geographical distribution of the release locations required for dose assessment, and hence MARFA is also used for geosphere transport calculations where coupling to one or more biosphere calculation cases is required.

Radionuclide transport in the biosphere will be calculated using the SNSHM and the landscape model implemented using the code Pandora (Section 4.4). Radiological consequences will be calculated using a model implemented in Matlab.

6.3 Flow modelling

The groundwater flow modelling for calculation cases supporting dose assessment is essentially the same as that supporting the probabilistic sensitivity analyses. In addition, however, EPM modelling will also be used to provide alternative estimates of the deposition hole flow rates, Q_F , and tunnel flow and EDZ rates, Q_{TDZ} and Q_{DZ} . This will allow an evaluation of the impact of model uncertainties associated with the choice of DFN or EPM representation. EPM modelling will also address density dependent flow and transient flow conditions.

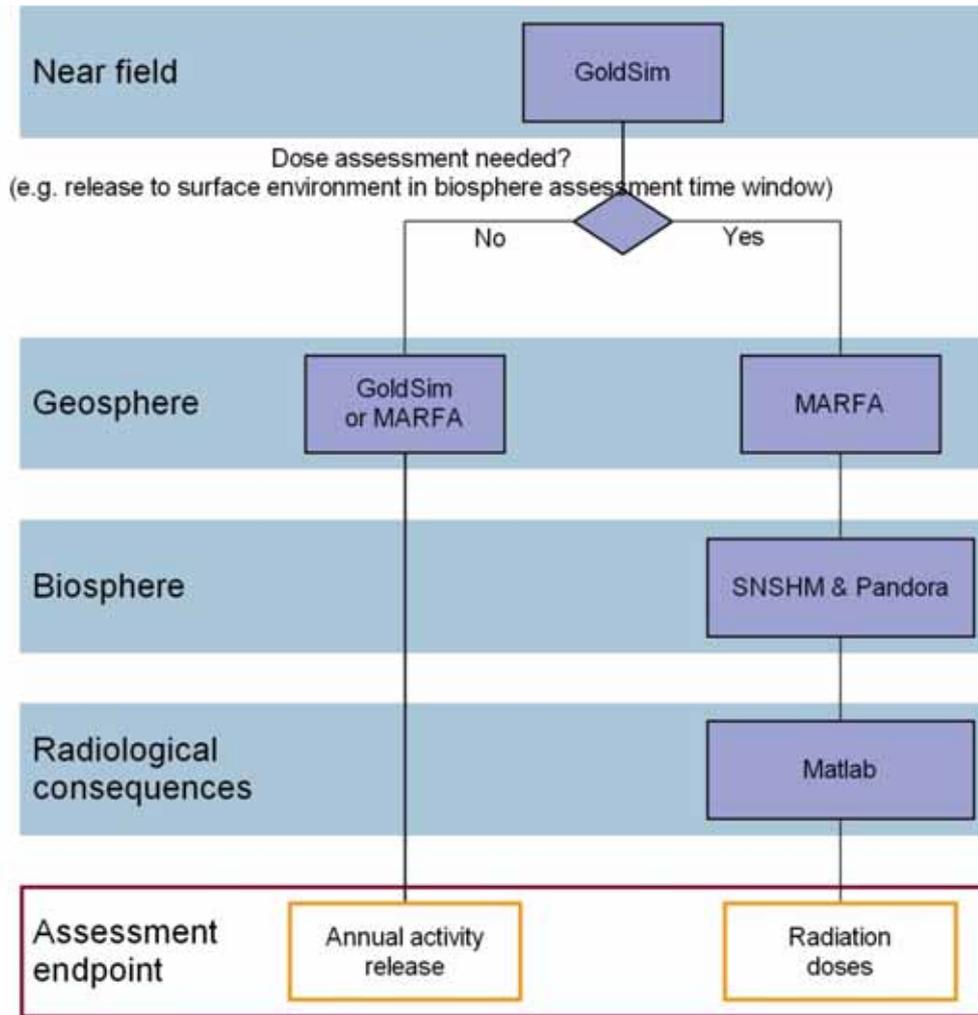


Figure 6-1. Transport model chains for analysis of calculation cases.

6.4 Deterministic analyses

Choice of reference location for defective canister

A reasonably pessimistic, reference location of a defective canister within the repository will be selected by means of the following procedure.

1. Divide the repository plane into a number (in the order of 10-20) of discrete 2-D elements (one way to do this would be, e.g. by means of a square grid - see Fig. 6-2, below - but this is just one or many possibilities).

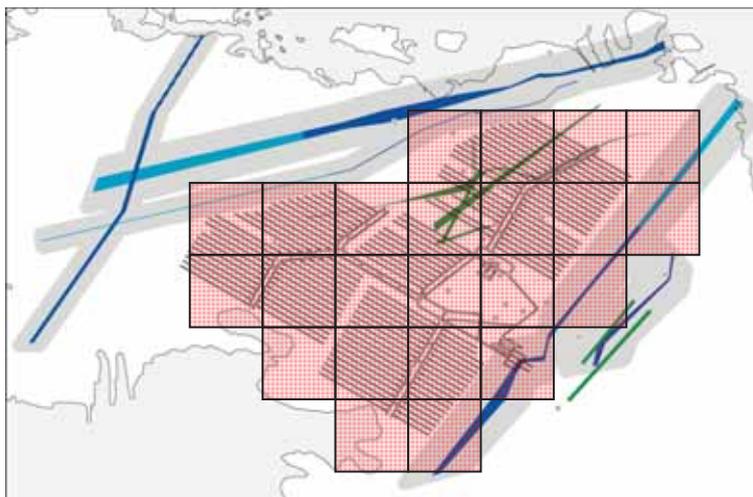


Figure 6-2. Possible division of the repository plane into discrete elements.

2. Use GoldSim to calculate near-field releases from a failed canister (single initial penetrating defect scenario) at the least favourable location in a given element of the repository plane, taking this position to be, for example, the canister location with the highest Q_F of each DFN realisation, but excluding any locations that do not satisfy the RSC. There will be as many GoldSim simulations as there are realisations per each repository element.
3. Take the GoldSim results for all repository elements (i.e. all failed canisters per realisation) and all realisations as input to MARFA calculations. There will be one MARFA calculation for the whole repository (all failed canisters) for each ConnectFlow DFN realisation.
4. From all MARFA calculations, calculate the ensemble statistics of the evolution of activity release in each geosphere/overburden interface element. In practice, assume equal probability for each realisation, which means that in the ensemble statistics can be calculated as a sum of all realisation divided by the number of realisations (i.e. weight of one realisation is $1/(\text{number of realisations})$).
5. Identify the repository plane element and canister position within that element giving the highest risk quotient (RQ) using either the Tier 1 or Tier 2 biosphere screening models (see Section 5.2 of Hjerpe et al. 2009) - *this is to be taken as the base case canister position for biosphere assessment.*

This last step is possible because MARFA provides a results file (results.dat) that includes the radionuclide name associated with each particle, as well as particle mass, arrival time, source ID and trajectory ID. The trajectory ID is the trajectory number of the CONNECTFLOW particle tracking simulation, i.e. each arriving particle can be linked with a flow path (including canister location and discharge location). Therefore, it is possible to determine the mass flux of a given radionuclide from a given canister location, even when releases from multiple failed canisters are modelled.

The effect of using other possible criteria for identifying the reference canister location in a given repository plane element (i.e. Step 2, above) will be considered. Alternatives to using the highest mean Q_F would be, for example:

- the highest mean Q_{TDZ} (averaged over all DFN realisations);
- the highest mean sum of Q_F and Q_{TDZ} ;
- the lowest mean WL/Q (averaged over all pathways from a given location and over all DFN realisations);
- the lowest individual WL/Q ;
-

If any of these alternatives yields a more pessimistic canister location from that found using Q_F , then the reference canister location may be revised accordingly.

It is clearly a cautious assumption to place the defective canister or canisters in the reference location defined above. This may be illustrated by calculating, in addition, the expectation value of releases of one or more radionuclides from the near-field or from the geosphere, assuming a defective canister to be randomly placed in the repository, and comparing this with the corresponding releases if the canister is placed at the reference location (note that a defective canister may occur with equal probability anywhere in the repository and the different DFN realisations are equally probable also).

Repository calculation cases

A number of GoldSim/MARFA calculations will be performed for the reference canister location and feed into the biosphere assessment. Important issues to look at will be, for example:

- considering individual DFN realisations - what is the variability in dose maximum between realisations due to a failed canister in the base case location (this can be assessed from the results of Step 3, above);
- sensitivity of dose to release/transport parameters (or lumped parameters) identified as important by simplified modelling and probabilistic sensitivity analysis;
- sensitivity to alternative model assumptions (e.g. colloid-facilitated RNT, ...).

Radionuclide transport in the biosphere

The strategy for radionuclide transport modelling in the biosphere assessment is addressed in detail elsewhere, and may be summarised as follows.

- The surface and near-surface hydrological model (SNSHM) will be run directly using MARFA output (without the need of first defining the landscape model) - see Section 6.6 for a description of the MARFA-SNSHM interface;
- SNSHM results (including activity out from the overburden) will be used as input to the delineation of the biosphere objects process in UNTAMO -thus, the information on where the activity enters the surface environment can be utilised

- when delineating the biosphere objects for the landscape model (this is a significant change compared with the previous strategy); and
- flows calculated using the SNSHM will be summed into aggregated flows for each object.

This means that radionuclide transport through the overburden will be modelled explicitly (unlike earlier Posiva safety analyses).

6.6 Data flows and interfaces

ConnectFlow-MARFA interface

MARFA allows direct coupling between flow and geosphere transport calculations. Two different approaches exist for the ConnectFlow-MARFA interface to handle the flow path information. MARFA 3.2.2, and prior versions, are based on fixed flow paths trajectories, but the flow rate and retention properties along each pathway may change in time. In MARFA 3.3, the trajectories of the flow paths are calculated within MARFA based on the node routing information from the ConnectFlow. The present plan is to use only MARFA 3.2.2 in the 2012 safety case.

The interfacing between ConnectFlow and MARFA 3.2.2 is implemented through a single file. ConnectFlow creates verbose pathline (PTV) files that are direct input to the MARFA (ConnectFlow is able to produce PTV-files that include pathline information from multiple DFN realisations; MARFA 3.2.2 assumes only one realisation per file).

GoldSim-MARFA interface

MARFA supports multiple sources and multiple geosphere pathways. In the stochastic full repository analysis, ConnectFlow provides canister specific near-field flow rates and also canister specific geosphere pathways as a ConnectFlow PTV-file. Near-field release rates through different near-field paths as they are simulated by GoldSim are linked with the corresponding canister specific near-field flow rate information. Interfacing programs are developed that couple the ConnectFlow geosphere pathways with the corresponding ConnectFlow near-field flow rates by a lookup table, and on the other hand, create MARFA source term file for the geosphere paths from the GoldSim release rates for the different canister specific near-field flow rates.

In addition to radionuclide release rates to be used by MARFA, GoldSim produces other output that can usefully be retained for documentation. In particular, as noted in Section 4.2, GoldSim calculates radionuclide concentrations within the transport and storage media as a function of time. Such output is useful, particularly for illustrating where in the multi-barrier system the bulk of the inventory of a given radionuclide resides, and how this evolves over time (see Fig. 6-3, which shows an example from the KBS-3H safety analysis).

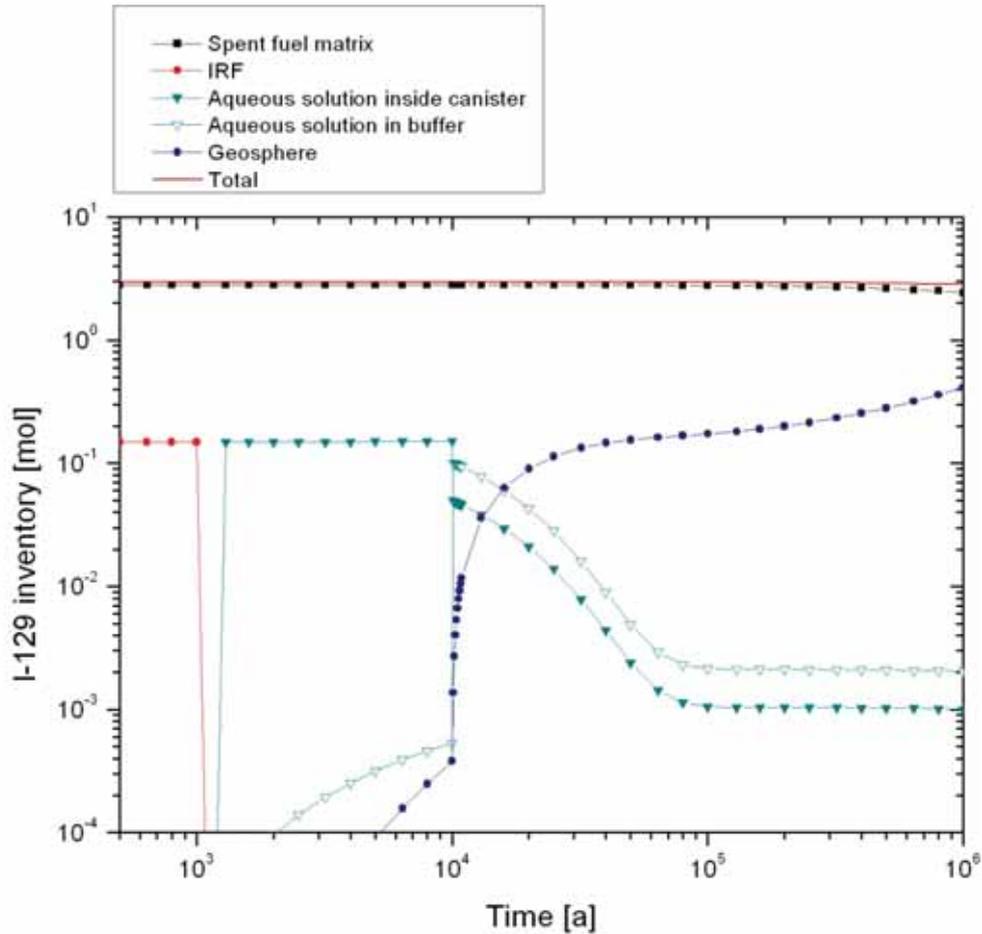


Figure 6-3. Distribution of I-129 inventory between different forms in the near field, and released to the geosphere, as a function of time (after Fig. B-2 of Smith et al. 2007).

Unlike release curves, such results can, for example, highlight the effectiveness of the fuel matrix at retaining the bulk of the inventory of safety-relevant radionuclides for a million years or more.

MARFA-SNSHM interface

MARFA/ConnectFlow is capable of delivering the activity release rates at the end of each individual transport path at its interface with the SNSHM (MARFA gives release rates and ConnectFlow provides transportpath trajectory information - these two data are linked by the number assigned to a transport path) as function of time. In addition, the related starting points and starting times are provided. This means that amount of data potentially fed to the SNSHM is large (for example, thousands of exit points per realisation of the DFN network, some tens of radionuclides and some tens of calculation cases).

However, the data can be reduced to a large extent by (i), combining all releases that occur to a given square element of the geosphere/overburden interface (current proposal is 10 m × 10 m) and (ii), using either a single DFN realisation or, alternatively,

providing ensemble statistics of the evolution of activity release in each geosphere/overburden interface element for all DFN realisations.

Thus, the main input to the SNSHM from geosphere transport modelling with MARFA is radionuclide-specific activity release rates as a function of time for square element of the geosphere/overburden interface. It is planned to deliver this input in time steps of 50 years over a time window taken to be the first 15 000 years. As noted in Section 4.3, MARFA provides a results file (results.dat) that includes the radionuclide name associated with each particle, as well as particle mass, arrival time, source ID and trajectory ID. The trajectory ID is the trajectory number of the CONNECTFLOW particle tracking simulation, i.e. each arriving particle can be linked with a flow path (including canister location and discharge location). Therefore, it is possible to determine the mass flux of a given radionuclide from a given canister location, even when releases from multiple failed canisters are modelled. The safety case can thus illustrate in one or more calculation cases exactly how each radionuclide travels from one or more failed canisters through the environment and causes potential exposure to humans and other biota.

It is also proposed to document the following MARFA output for use in biosphere modelling:

- radionuclide-specific activity release rates as a function of time, summed over all elements of the geosphere/overburden interface; and
- cumulative radionuclide-specific activities as function of time, summed over all elements of the geosphere/overburden interface.

These two results may be used as direct input into the screening models used in the biosphere assessment 2009 (the strategy for radionuclide screening for the 2012 safety case has yet to be fixed).

7 ANALYSES OF SCENARIOS WITHOUT CONSEQUENCES IN DOSE ASSESSMENT TIME WINDOW

For scenarios and calculation cases in which no radionuclide release to the biosphere occurs in the biosphere assessment time window, only spatially integrated releases across the geo-bio interface are required to assess compliance with regulatory geo-bio flux constraints (see Section 1.2). Hence, in most cases, GoldSim will be used to calculate both near-field release and transport and geosphere transport (Fig. 7-1).

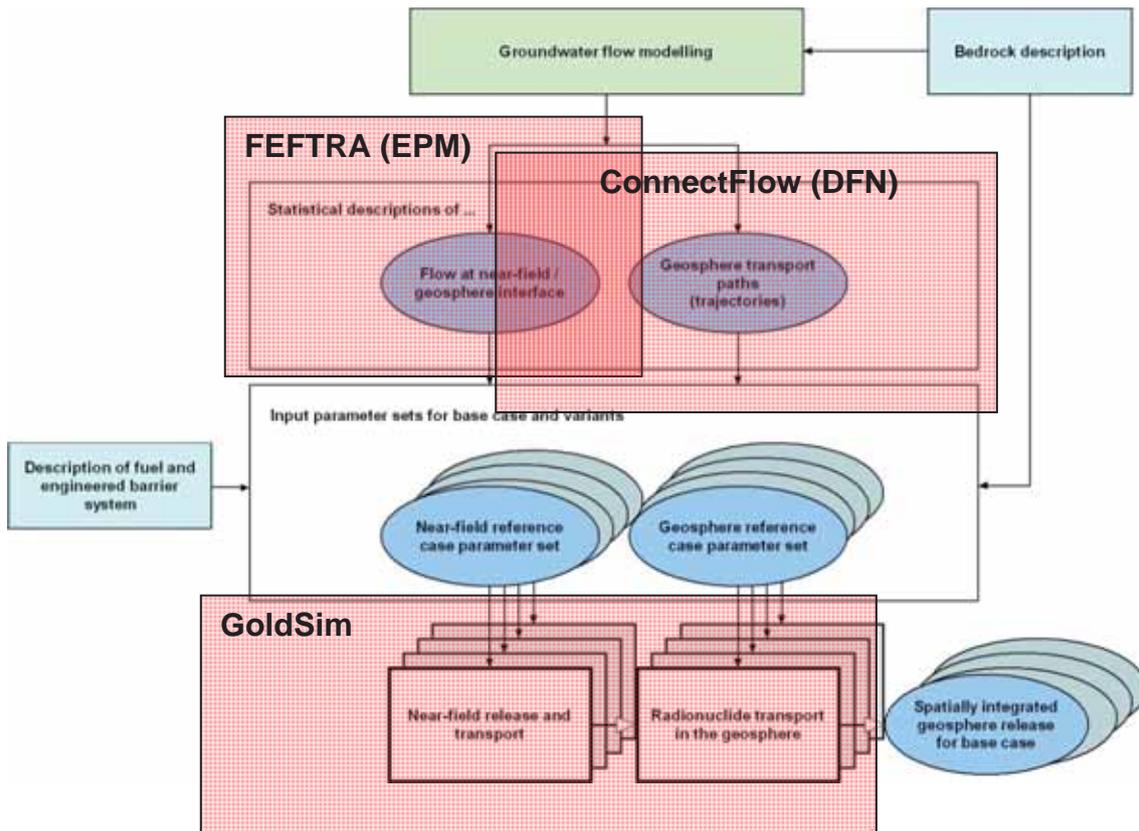


Figure 7-1. Model chain for deterministic calculations supporting the evaluation of geo/bio fluxes.

The model chain will be essentially the same as that used for probabilistic sensitivity analyses (Section 5.2 and Fig. 5-1). Again, GoldSim will be used to model near-field release and transport and geosphere transport along the transport paths from a failed canister location to the biosphere, represented by three representative geosphere release paths (see Fig. 5-3) (or small number of paths, each characterised by a transport resistance, WL/Q).

Flow modelling will produce stochastic and spatially varying descriptions of the flow at the near-field/geosphere interface and of the geosphere transport paths (Table 5-1). However, unlike the probabilistic sensitivity analyses, single values of each of these flow parameters will be selected for each deterministic calculation case. The selection

will be made by expert judgement, and will depend, in part on the mode by which the canister fails and how this is expected to be correlated (or not) with canister location.

In the case of canister failure by corrosion, canister failure is most likely at high-flow locations in the rock, and calculation cases addressing this mode of canister failure are likely to employ WL/Q values chosen mostly from the low end of the distribution (the yellow line in Fig. 4-3), in line with the regulatory requirement that the analysis does not overestimate the performance of safety functions or underestimate radiological consequences (see Ch. 1). The annual activity flux to the biosphere in this case, assuming N relatively high-flow locations where the canisters fail by corrosion in a million year time window, will be calculated according to the equation:

$$G(t) = \sum_{j=1}^N G_j(t_j^{FAIL}, t), \quad (7-1)$$

where t_j^{FAIL} is the canister failure time calculated for a canister in deposition hole j (taking into account the specific hydrogeological properties of the rock around this hole) and $G_j(t_j^{FAIL}, t)$ is annual activity flux at time t from a canister in deposition hole j failing at time t_j^{FAIL} .

In the case of canister failure due to rock shear, the corresponding equation for the annual activity flux to the biosphere is:

$$G(t) = \int_0^t P(t') G(t', t) dt', \quad (7-2)$$

where $P(t')$ is the canister failure frequency at time t' and $G(t', t)$ is the annual activity flux at time t from a canister failing at time t' due to rock shear. Note that any rock shear event that causes canister failure may also significantly perturb transport properties of the rock. A cautious approach to geosphere transport will be taken in such cases in which the geosphere transport resistance will be set to a low value, irrespective of the location of the failed canister in the repository. The details of this approach are yet to be decided.

MARFA may also be used for some geosphere transport calculations. The choice of model chain will depend on the specific case to be analysed. For example, MARFA has the capability of dealing with geosphere transport in a transient flow field arising, e.g. due to the presence over the repository of a moving ice front. Groundwater flow analysis for cases that involve significant transient or density dependent couplings of the flow field will be performed using FEFTRA model and EPM approach. Simulation results of the FEFTRA modelling gives estimated on the magnitude of the flow transients around the repository and deposition holes and in the bedrock along the release paths. These simulation results combined with the base case simulations results (e.g. ensemble means?) will be used i) to create time dependent near field flow rates for the GoldSim to calculate the near field release rates and ii) to generate time dependent flow rate along the representative geosphere release path for the transient MARFA simulation. This analysis is not addressing the range of different release paths and canister locations, but mainly rather the transient behaviour of the overall (mean) conditions.

8 IMPLEMENTATION AND DOCUMENTATION OF CALCULATIONS

8.1 Quality measures

Quality measures are to be applied (or are being applied) in the development and application of models and data, as well as the computer codes that are used to solve the governing equations of the models. Quality measures relating to the implementation and documentation of calculations, as prescribed in the Safety Case Plan (Posiva 2008), include:

- documentation of input for the production runs;
- application of a procedure to ensure codes are correctly applied;
- documentation of the code versions used; and
- reporting of non-conformities.

The planned procedures to implement these quality measures are given in the present chapter.

There are also additional quality measures given in the Safety Case Plan, namely:

- validation of input data for the scenarios and models considered; limits of applicability of input data are checked against assumptions related to scenarios and models;
- validation of the models used to analyse the scenarios;
- verification of assessment codes; and
- validation of the assessment codes for the intended application.

These quality measures will be reported elsewhere, including in the Models and Data Report and in the Analysis of Scenario Report, where needed.

8.2 Implementation of calculations

The general procedure foreseen for implementing calculation cases is illustrated in Fig. 8-1, taking the example of a calculation case analysed using GoldSim for near-field release and transport and MARFA for geosphere transport.

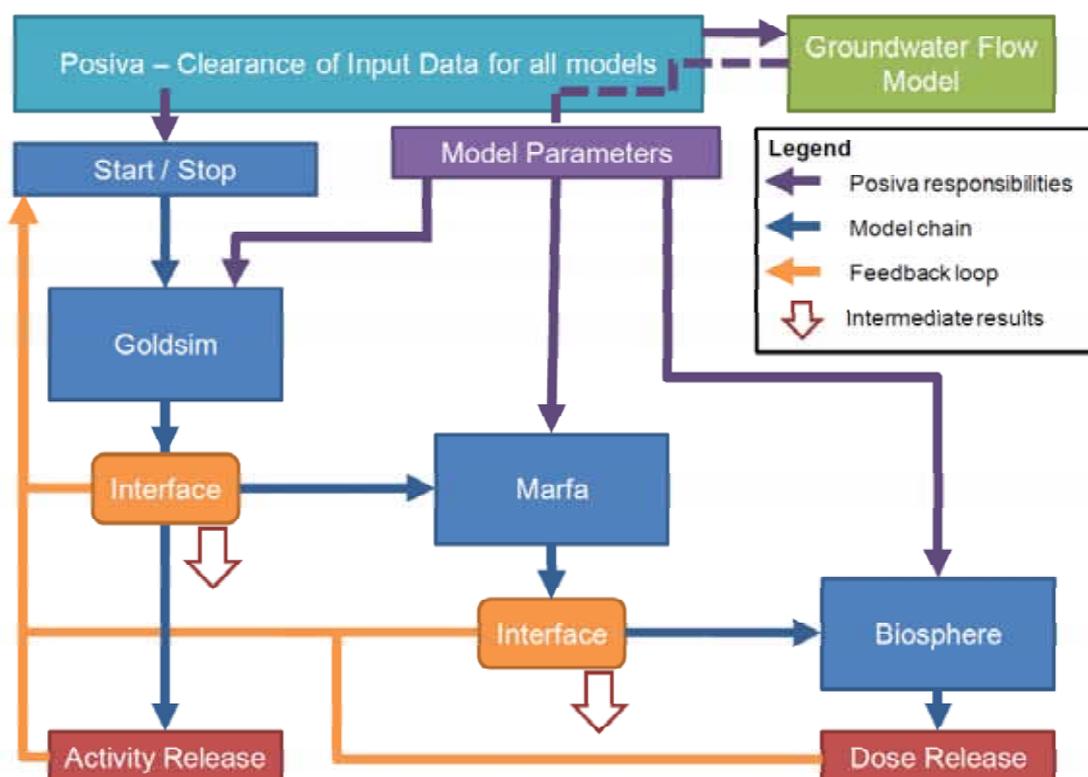


Figure 8-1. General procedure foreseen for implementing a calculation case. "Posiva responsibilities" is to be understood as responsibilities of SAFCA.

The procedure consists of the following steps:

1. Posiva (SAFCA) clears a calculation case with its classification (e.g. as sensitivity case, "what-if?" case, or complementary cases), input parameter values and models for the near-field, geosphere and biosphere. This includes all data and parameters entering the model chain from beyond and includes the input data from the groundwater flow model⁷. SAFCA attaches a version number to these data.
2. SAFCA communicates the initiation of the model chain.
3. The input data coming from SAFCA specifically for the GoldSim model receives a version number and the GoldSim models for near-field and geosphere are run (input file generation and versioning are described in Section 8.3). The results are forwarded to the first interface.
4. At the first interface the GoldSim results are processed according to the procedure described in Section 8.4. In case of non-conformities, the model chain is stopped. SAFCA will need to reconsider and clear the calculation case again (return to step 1). The activity release from the geosphere is processed as a result of the model chain and output with the same version number as the GoldSim input data. If dose assessment is not required, the model chain ends here.

⁷ The groundwater flow model is not part of the model chain described here but provides necessary input for the model chain. The input data used for the groundwater flow model must also be cleared.

Otherwise the input data for the MARFA model is generated and forwarded with the version number of the GoldSim input data.

5. The MARFA model receives the input from the first interface and needed additional model parameters. The input data as a whole is assigned a version number. Then the MARFA model is executed and the results are forwarded to the second interface.
6. At the second interface, the MARFA results are processed according to the procedure described in Section 8.4. In case of non-conformities, the model chain is stopped. SAFCA will have to evaluate the non-conformities, and reconsider and clear the calculation case again. Eventually, either the whole model chain is re-executed from the beginning (return to step 1) or only the MARFA model is re-run (return to step 5). Otherwise, the results of the MARFA model are output as an intermediate result with the version number of the MARFA input data, and the input data for the biosphere modelling is generated and forwarded.

The following additional steps, which concern dose assessment, are not shown explicitly in Fig. 8-1, but are contained implicitly in the box labelled "biosphere".

7. The surface and near-surface hydrological model (SNSHM) receives the input from the second interface, together with the additional parameter values needed by this model. The input data as a whole is assigned a version number. Then the model is executed and the results are forwarded to the third interface.
8. At the third interface the results of the SNSHM are processed to generate the output in terms of environmental radionuclide activity concentrations and are checked for non-conformities. The output is assigned the version number of the used input data. In case of non-conformities SAFCA has to evaluate the non-conformities, and reconsider and clear the calculation case again: The model chain restarts at steps 1, 5 or 7. Otherwise the output is processed further in conjunction with the UNTAMO modelling output (the evolution of the surface environment; this modelling is carried out separately).
9. The UNTAMO modelling output receives the input from the third interface. Then the combination is used to delineate the biosphere objects (BSO) and the results are forwarded to the fourth interface.
10. At the fourth interface, first the delineated BSO are applied in the SNSHM model to calculate the aggregated flows for each biosphere object. Then, the results of the SNSHM and UNTAMO are processed in the Pandora model to generate the output in terms of environmental radionuclide activity concentrations. The output is assigned the version number of the used input data. In case of non-conformities SAFCA has to evaluate the non-conformities, and reconsider and clear the calculation case again: The model chain restarts at steps 1, 5, 7 or 9. Otherwise the results are forwarded to the fifth interface.
11. At the fifth interface, the dose calculation models (for humans and other biota) receive the input from the fourth interface, together with the additional parameter values needed by these models. The output is assigned the version number of the Pandora input data. In case of non-conformities SAFCA has to evaluate the non-conformities, and reconsider and clear the calculation case again: The model chain restarts at steps 1, 5, 7 or 10. Otherwise the model chain ends.

8.3 Input file generation and version management

The input data for each calculation case consists of near-field and geosphere model parameter values and other input, e.g. data calculated from other models, such as groundwater flow modelling, and numerical (discretisation) parameters (types of input parameters and the selection of values are described further in Section 8.5). As long as no changes are made to the models, the associated computer codes or the input parameters, the output of any one calculation case is perfectly reproducible.

In practice the input parameter values may be modified, e.g. model parameters are changed or calculated data from other models is updated. A common way of keeping track of safety assessment calculations and maintaining the reproducibility of calculation results is the implementation of a version management system (VMS). Each version of each element defining a calculation case – the model, the model code and the input data – and the calculation case itself are assigned unique identifiers (version numbers). The output produced for a calculation case receives the version number of the calculation case. *Any change in a file requires that a new version number is assigned to the file.*

It is planned to use Excel workbooks to manage the efficient execution of calculation cases. These workbooks will be used to produce and organise all near-field and geosphere input data for each calculation case. They consist of:

- a table of all calculation cases with their defined and selected individual parameter sets;
- a database to manage raw data, reference files (see below) and cleared data in data tables;
- a pre-processor to automatically generate code-specific input files using the table of calculation cases and the database;
- a "compare" tool to visualise differences between input data for different calculation cases; and
- an integrated VMS for the input files produced.

These workbooks are expected to make it possible to produce and manage input files in a traceable manner and with a high degree of accuracy and efficiency.

In practice, many input parameter values are common to most or all calculation cases. Thus reference files containing these parameters can be used as a basis for input file generation. *All reference files and inputs must be checked manually. These checks must be documented.* The files for additional cases can be checked by comparing the new files and inputs with the reference files electronically; *these checks must also be documented.*

8.4 Interface data exchange management

Each interface between one mode/computer code and the next in the chain comprises several programs or procedures for various purposes concerning data flow and processing (Fig. 8-2):

- output of previous model: output data (i.e. calculation results) from the previous model is read and processed;
- intermediate results - the calculation results from the previous model are made available in a format suitable for QA and documentation purposes (see Section 9.6);
- feedback for model chain - feedback drawn from the processed data is provided to the modellers who use it to check the output of the previous model for plausibility and any kind of non-conformity. If necessary, the modellers stop the chain; and
- input for next model - the output of the previous model is processed to become part of the input for the next model.

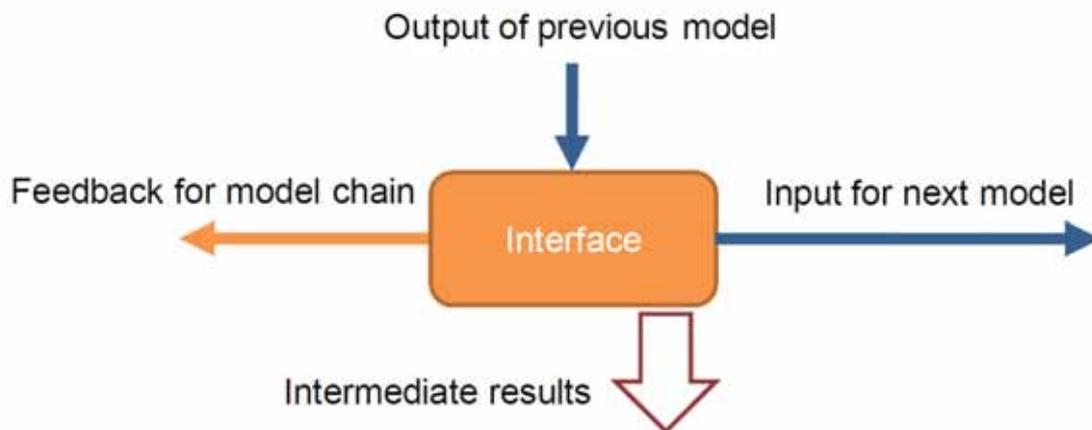


Figure 8-2. Schematic illustration of input/output at a model interface.

To standardise and monitor data exchange at the interfaces between the different models, it is planned to implement a simple but comprehensive interface data-exchange management system that will cover at least the interfaces between GoldSim and MARFA and between MARFA and the biosphere (landscape) model.

An interface data-exchange management system serves the following purposes:

- allow a standardised file exchange between models, i.e. defined (processed) model input data and outputs are uploaded on a server;
- version documentation of defined calculation results;
- simple automation of communication, e. g. an upload of a new calculation output is communicated to modellers who need this output as input.

Each of the main interfaces is discussed in more detail in the following sections.

The modellers will need to describe the data formats for data exchange across each interface, and SAFCA needs to identify which additional intermediate results will need to be documented (some first suggestions are given in the following sections). From these descriptions, the input / output conversion functionalities of the interfaces will be derived

Other interfaces may be less amenable to such a system, relying to some extent on expert judgement to derive input parameters from one code from the output of another. Here, it is critical that the rationale for such judgements be fully and traceably documented.

8.5 Selection of input parameter values

Types of input parameters

Groundwater flow and radionuclide transport models require the specification of parameters of a number of different types:

- parameters describing the initial state of the repository system, including geometrical parameters, spent fuel types and burn-ups, radionuclide inventories and partitioning;
- parameters describing the evolution of the repository system and its safety functions, including e.g. the nature and number of canister failures, the evolution of the transport resistance provided by a penetrating defect in a canister, and the evolution of groundwater flow and geochemical conditions;
- parameters characterising radionuclide release and transport processes under these evolving conditions; and
- parameters controlling, e.g. numerical discretisation of time and space.

Many of the parameter values will be set based on data ranges that will be given in the Models and Data Report. The values assigned will, in some cases, depend on the conceptual models for repository evolution and radionuclide release and transport (e.g. if it assumed that there is some disturbance to the buffer/rock interface, this will affect the setting of the parameter Q_F). Other parameters, such as the nature and number of canister failures and the evolution of the transport resistance provided by a penetrating defect in a canister, will be based on supporting analyses, including qualitative considerations and scoping calculations. In some cases, as described below in the case of data related to flow, site-specific data has to be refined or processed in some way in order to derive parameters for groundwater flow and radionuclide transport models.

Use of site-specific data to derive parameters for groundwater flow modelling

The hydrogeological structural model describes two-dimensional zones embedded in a three-dimensional model volume. In essence, the transmissivity of the (two-dimensional) hydrogeological zone is the same as the hydraulic conductivity of the three-dimensional formation.

The starting point of determining the transmissivity of the hydrogeological zone is its (modelled) intersections with the drill holes. Thereafter the intersections are treated one

by one. At one such intersection, all substantial transmissive fractures are interpreted as belonging to the hydrogeological zone. In most cases, there are only one or two transmissive fractures dominating the groundwater flow. Next, these separate fracture transmissivities are summed to yield the transmissivity of the hydrogeological zone at the intersection with the drill hole. For the site-scale flow model it is then assumed that the geometric mean of the transmissivities at the drill-hole intersections represents the effective value of the whole hydrogeological zone.

After associating these specific measured transmissivities with the hydrogeological zones, the remaining transmissivities are interpreted as being associated with the sparsely fractured rock mass, lying between the hydrogeological zones. In the EPM approach, the bedrock outside the deterministic zones is divided into depth classes and the average hydraulic conductivity is calculated for each drill hole.

Discrete fracture network (DFN) modelling describes the rock mass by building the model from individual fractures. The model is based on a stochastic approach, in which the properties of the fractures are described by statistical distributions. The model of fracturing is based on the geological description of the fractures (Olkiluoto Geo-DFN model). The hydraulic properties of the fractures are calibrated using data from the hydraulic tests performed in the drill holes.

The approach combines a deterministic representation of the hydrogeologically-active deformation zones with a stochastic representation of the less fractured bedrock outside these zones, using a hydrogeological discrete fracture network (Hydro-DFN) concept. Hydraulically, the HZ and Hydro-DFN models are parameterised with data from the single-hole Posiva Flow Log (PFL) pumping tests to calibrate the connectivity of the Hydro-DFN model and to parameterise the fracture transmissivity distributions. Fracture size parameters are determined in the Hydro-DFN flow simulations by matching the simulated and measured PFL fracture intensities.

An essential part of the groundwater flow analyses is calibration, which strives to ensure that the flow model corresponds to the hydraulic characteristics of the real system as much as possible.

Numerical parameters

In numerical modelling, the density of spatial discretisation and the size of the time steps used can affect the accuracy of the results if they are insufficiently fine.

The numerical resolution in the site scale groundwater flow analysis is usually a compromise between memory/time constraints of the computer and the scale of the details that are represented in the model. Numerical accuracy of the solution is confirmed by examining convergence of the solution, calculating mass balance over the solution, checking the range of the head/pressure solution taking into account the boundary conditions and by calculating also possibly other e.g. head dependent measures for the goodness of the solution. Both ConnectFlow and FEFTRA are able to increase spatial resolution of the model around the most important regions of the model, like the repository.

The effect of the choice of numerical parameters when modelling near-field release and transport using GoldSim has been investigated in Pulkkanen & Nordman (2010). The results show that discretisation has a minor effect on results within the numerical parameter ranges considered. GoldSim uses a Laplace transform method for geosphere transport modelling, so spatial discretisation is not an issue. In the 2012 safety case, the effect of time step length will be analysed for some calculation cases (see code verification report).

MARFA is based on the particle tracking in the time-domain. The output of the model is particle residence times in the model, i.e. it does not directly produce breakthrough curves of the nuclides. Calculation of the breakthrough curves from the particle residence times includes a source uncertainty, but the possible uncertainty breakthrough curves can be easily checked by varying the post-processing parameters of the MARFA. Statistical accuracy of the results can be analysed by changing the number particles used in the simulation.

8.6 Documentation of output

Documentation of safety assessment calculations in a comprehensive and traceable manner⁸ while retaining transparency in the project reports is an issue of major importance. There are too many results for it to be reasonable of useful to include all of them in the main project reports. It is, however, desirable that results and their associated input files are readily available to safety assessors for inspection and archived for future reference.

It is planned to develop an electronic system *docgen* to keep track of, and to archive, the results of safety assessment calculations in a model chain as they are produced. In this way, SAFCA will be able to follow the progress of the calculations and do quality assurance and plausibility checks in a timely manner. The documentation will be generated automatically as soon as a model run has finished successfully. Data for the model run will also be pre-processed and stored on a server automatically. Any authorised user will be access it with a web browser.

The documentation of a calculation case will consist of a webpage with links to the following:

- all input files and identifiers of all models used in the model chain to run the calculation case;
- visualisations of selected results of time series (for e.g. release vs. time) in the browser as figures or tables. In order to focus on aspects of interest, the following features of the figures may be customised interactively:
 - scaling of axes;
 - selection of items (e.g. specific radionuclides) shown; and
 - units of axes, e.g. release rates in Bq a^{-1} or mol a^{-1} ;

⁸ See requirement for traceability in Guide D.5, Para A1.10, referred to in Ch. 1.

Because documentation will be produced according to the same standard for all calculation cases, quality assurance will be facilitated. The post-processing and documentation of all calculation cases will be completed as soon as the last model run is processed. The documentation produced in this way can be stored offline on a CD and selected material can be added to a printed report. To this end, it is intended that the visualisation of results will be flexible, in terms of scaling of axes, tiles, selection of items etc., and will be able to export graphics in a format with sufficiently high quality for printed reports.

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