Integrated System Model (ISM) Theory Manual

NWMO-TR-2022-07 R002 **March 2025**

M. Gobien, A. Boyer, S. Briggs and C. Medri
Nuclear Waste Management Organization

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Document History

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Revision Summary

Revision Number	**Date**	**Description of Changes/Improvements**
R000	2023-03	Initial issue
R001	2024-01	Revised document to align with ISM v1.3.
R002	2025-03	1. Revised document to align with ISM v1.4, specifically the addition of ISM-WF v1.0 model (See Chapter 3) and making ISM-NF an optional component of ISM (see Appendix A) 2. Retired versions of the ISM models representing the South Bruce Site following the site selection decision and removed South Bruce Site related content from the ISM theory manual

ABSTRACT

Title: **Integrated System Model (ISM) Theory Manual**
Report No.: **NWMO-TR-2022-07 R002**
Author(s): M. Gobien, A. Boyer, S. Briggs and C. Medri
Company: Nuclear Waste Management Organization
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Abstract

This report describes the theory for the Integrated System Model (ISM). The ISM is intended to assess radionuclide and element transport and dose as a part of post-closure safety of a deep geologic repository for used fuel. The system model is composed of a series of linked models representing the wasteform, the geosphere and the biosphere.

As part of ISM v1.4, the wasteform model (ISM-WF) is newly developed and one of the three required components of the ISM. The ISM-WF model estimates radionuclide and element “source terms” from a variety of wasteforms that may be disposed of in the deep geologic repository (DGR) (e.g., CANDU fuels, prototype and research fuels, and DGR facility generated low level wastes). The wasteform model interfaces with the geosphere model by passing source term fluxes to the geosphere.

As of ISM v1.4, the near-field model (ISM-NF) becomes an optional component as its primary use is replaced by the ISM-WF. It may be used for benchmarking, validation and scenario dependent purposes. The ISM-NF consists of the wasteform, containers, engineered barrier system, and excavation damaged zone surrounding the placement room. The near-field model assumes failure of containers and models degradation of the used fuel, and transport of contaminants (radionuclides and chemical elements) from the failed containers, through the engineered barrier system, through the excavation damaged zones and into the intact host rock. The near-field model can interface with the geosphere model by passing the integrated fluxes of contaminants entering the geosphere at one of a few predefined interfaces. For example, the interface between the excavation damaged zone and the intact rock.

The geosphere model (ISM-GEO) describes the movement of contaminants from the repository via the groundwater in the rock mass and geosphere features (e.g., fractures, aquifers) to the surface environment. The source term in the geosphere model is determined by the wasteform model. The geosphere model interfaces with the biosphere model by passing integrated fluxes of contaminants to a domestic water well, as well as to predefined aquatic and terrestrial discharge areas at surface.

The biosphere model (ISM-BIO) describes the movement of contaminants between surface water, soils, atmosphere, vegetation, animals and humans. The biosphere model estimates concentrations of contaminants in environmental media (soil, sediment, groundwater, surface water and air). Based on the environmental media concentrations, the model estimates the radiological dose to a variety of receptors assumed to be living near the repository.

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1. INTRODUCTION

1.1 Context

The Nuclear Waste Management Organization (NWMO) is responsible for the long-term management of Canada’s used nuclear fuel. The planned approach includes placement of the used fuel in a deep geological repository (DGR). The NWMO has selected the Wabigoon Lake Ojibway Nation-Ignace Area (also referred to as the Revell Site) as the site for the DGR.

To support development of the licensing application for the DGR a safety case is being assembled to demonstrate the safety of the DGR facility at the selected site and the meeting of all applicable regulatory requirements. A key component of the safety case is the long-term evaluation of safety, also referred to as the post-closure safety assessment. This is an assessment that examines potential long-term consequences of a repository (radiological and otherwise) to future humans and the environment. The post-closure safety assessment considers timeframes from closure of the repository until well into the future (typically 1 million years or greater). Post-closure safety assessments require a broad range of inputs to support a variety of numerical modelling efforts used to quantify analysis end points and assess the impact of the repository. Post-closure safety assessment end points include:

- radiological dose to humans and environment (e.g., plants and animals); and
- concentration of contaminants in environmental media (e.g., surface waters, groundwater, soil, sediment and air).

Models developed to assess these endpoints include the Integrated System Model (ISM), the Non-human biota model (Medri and Bird, 2015) and the Human Intrusion Model. Model inputs include data describing the used fuel, engineered barrier system, repository design, geosphere, biosphere as well as human lifestyle and dose model data. Figure 1-1 illustrates the relationship between the input data, models and post-closure analysis end points.

This report describes the ISM theory and governing equations for version 1.4. The ISM is the primary tool used to assess liquid-mediated contaminant (radionuclide and element) transport from the used fuel to the biosphere. The ISM estimates environmental media concentrations and dose consequences to a variety of receptors. To the extent possible the ISM is informed by the currently available repository design and site characterization data and models. However, some components of the ISM remain generic or simplified due to the lack or preliminary nature of some of the supporting design and site data. Over time the ISM will be iterated to include additional site-specific features, processes, and data.

The current implementation of the ISM consists of three required component models, the wasteform (ISM-WF), geosphere (ISM-GEO) and biosphere (ISM-BIO) each built using commercially available software programs: AMBER (Quintessa 2023) for ISM-WF and ISM-BIO, and HydroGeoSphere or HGS (Aquanty 2015) for ISM-GEO. The near-field (ISM-NF) from version 1.3 and earlier of ISM remains as an optional component. A custom linking and data management tool, paLINK, has also been developed to automate execution of the ISM component models, preprocess data, pass data between component models and post-process outputs. While paLINK can be used to run ISM component models individually or automate ISM execution, it does not container any physics so is not described in the theory manual (this document). Figure 1-2 illustrates the connections between the various ISM components.

A high-level description of the DGR concept modelled by the ISM is provided in Section 1.2 and the scope of this document is provided in Section 1.3.

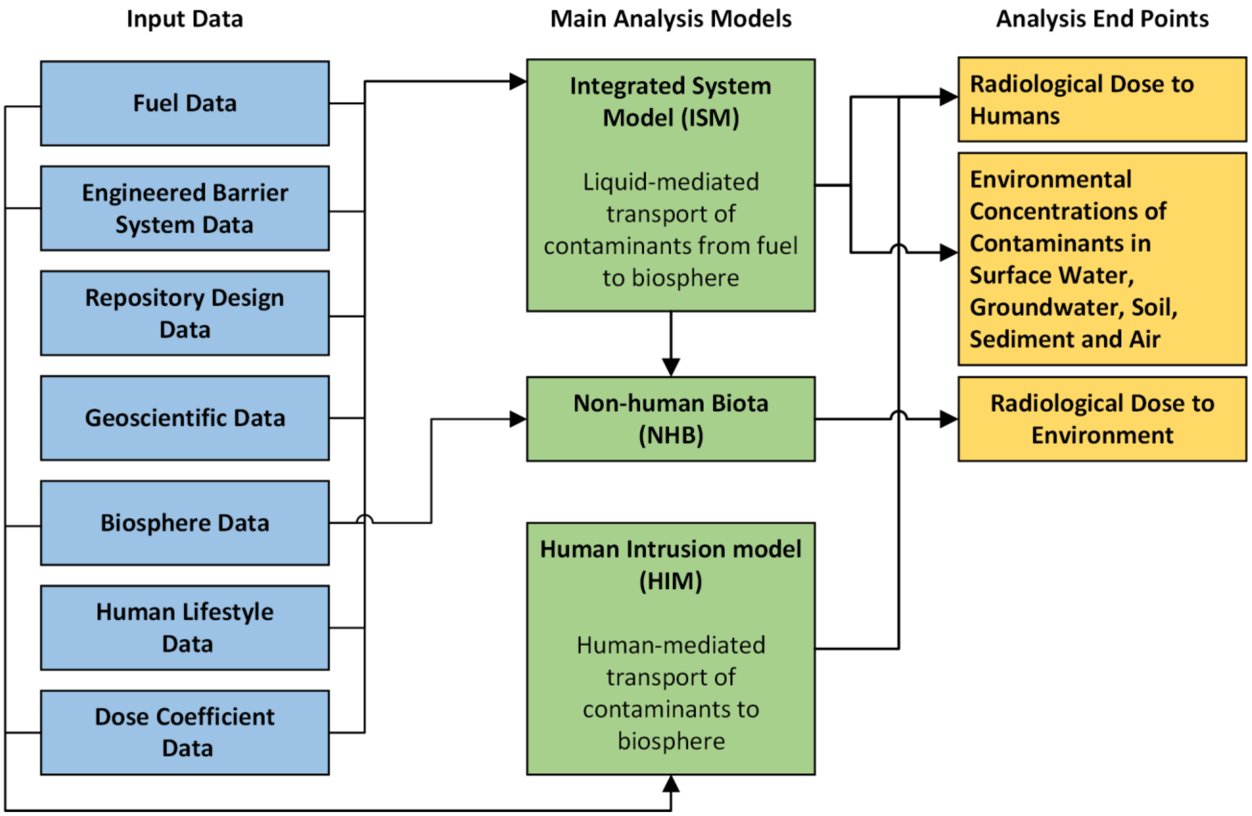

Figure 1-1: Illustration of Post-closure Safety Analysis Input Data, Models and End Points

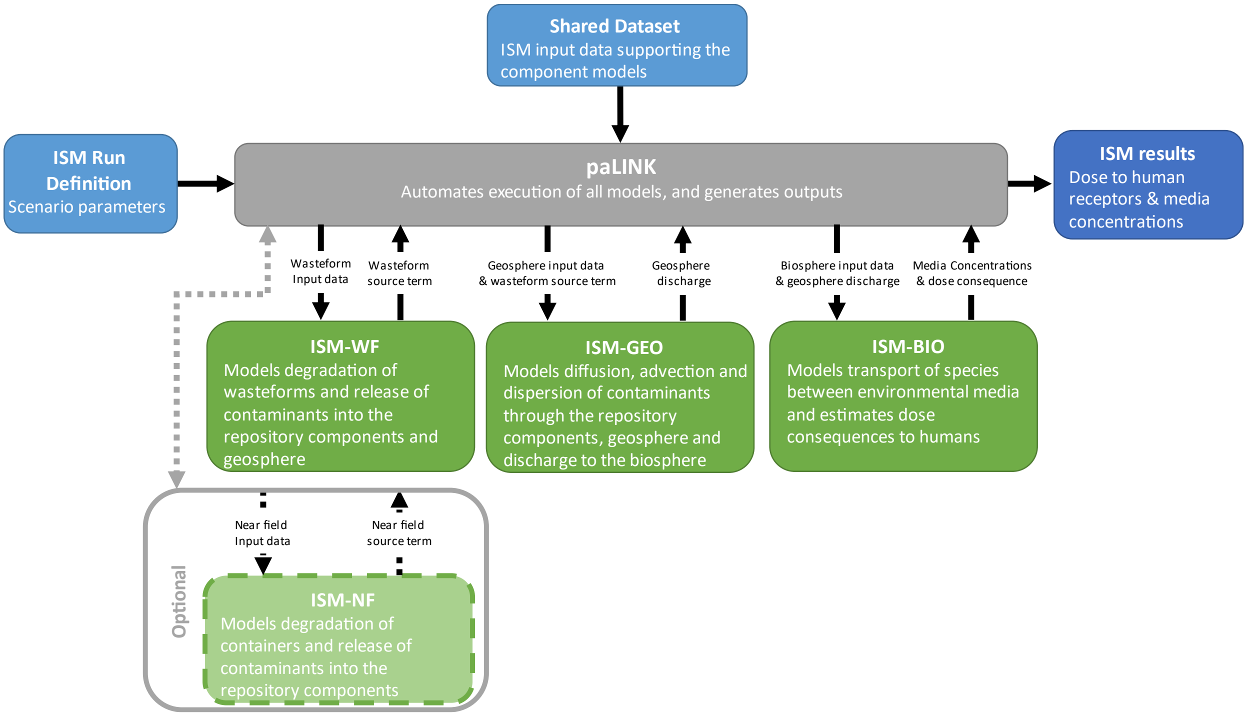

Figure 1-2: Illustration of ISM Inputs, Components and Outputs

1.2 Description of the DGR System

A DGR is a multiple-barrier system designed to safely contain and isolate used nuclear fuel over the long term. The reference repository is planned to be located approximately 500-800 metres below the ground surface. The final depth will depend upon the specific geology and detailed characteristics of the site. It consists of a network of placement rooms for the used-fuel containers and clay-based sealing systems, as well as a series of access tunnels and shafts to ensure accessibility and monitoring. The layout of the repository will depend on a number of factors, including the characteristics of the host rock, refinements made to the final design of the engineered-barrier system, final safety considerations, and the inventory of used fuel to be managed.

The used fuel containers are encased within a bentonite buffer box which will be placed horizontally in the placement rooms. Spaces between individual buffer boxes will be filled with highly compacted bentonite blocks while gaps between the buffer boxes and spacer blocks and the excavation wall will be filled with bentonite pellets called gap fill. Concrete and clay-based bulkheads will be placed at strategic locations in tunnels and shafts and at the entrance to each placement room.

Figure 1-3 illustrates the generic repository concept.

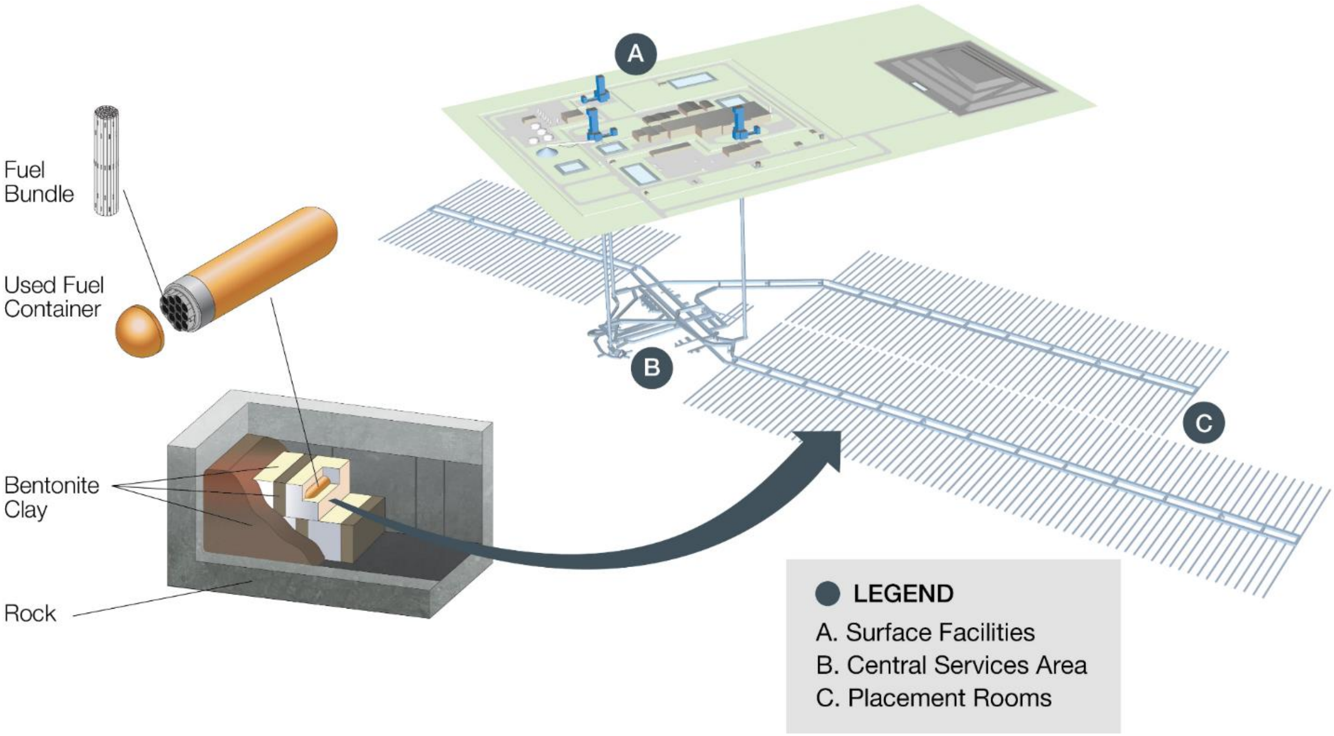

Figure 1-3: Illustration of the Multi-barrier Concept for a DGR

1.3 Scope of this Report

This report describes the model theory and equations governing in the ISM as well as the underlying assumptions. The report contains four main Chapters:

- Chapter 2 – Waste Inventory and radioactive decay;
- Chapter 3 – Wasteform model theory;
- Chapter 4 – Geosphere model theory; and
- Chapter 5 – Biosphere model theory.

Chapter 2 of this report describes the inventory of fuel expected to be stored in the DGR, the basis for the contaminant inventory in the fuel, and the theory and equations associated with radioactive decay and ingrowth as implemented in the ISM-WF, ISM-GEO and ISM-BIO models.

Chapter 3 describes the theory and equations associated with the ISM-WF model. This model assumes used fuel containers have failed at some point in the future and models the degradation of the fuel. The ISM-WF model estimates radionuclide and element “source terms” from a variety of wasteforms that may be disposed of in the deep geologic repository (DGR) (e.g., CANDU fuels, prototype fuels and research fuels, and DGR facility generated low level wastes). The wasteform model interfaces with the geosphere model by passing source term fluxes to the geosphere.

Chapter 4 describes the theory and equations associated with the ISM-GEO model. This model receives integrated flux of contaminants from the ISM-WF model and models the sequent transport of contaminants from the repository to the surface environment via the groundwater transport through the rock mass and other geosphere features (e.g., fractures and aquifers).

Chapter 5 describes the theory and equations associated with the ISM-BIO model. This model receives the integrated flux of radionuclides and stable isotopes from the ISM-GEO model and determines the concentration of contaminants in environmental media (e.g., surface water, groundwater, sediments, soils, and air) and estimates the radiological dose to a variety of lifestyles.

Appendix A describes the theory and equations associated with the ISM-NF model. This model assumes used fuel containers have failed at some point in the future and models the degradation of the fuel, release of contaminants from fuel and the subsequent transport of contaminants through the engineered barrier system, excavation damaged zone, and into the geosphere.

Throughout this report variables applicable to radionuclides and elements are referred to as contaminants and are denoted with the subscript or superscript j. Variables only applicable to radionuclides are denoted with subscript or superscript i. Variables applicable to elements (meaning the sum of all isotopes of a given element) are denoted with subscript or superscript k.

This report is intended to document the ISM theory as currently implemented in version 1.4. Excluded from this report are:

- Numerical solution techniques;
- Data for the ISM parameters;
- Use of data management and ISM linking tool paLINK;
- Identification and rationale for the processes considered; and
- Post-closure safety assessment scenarios.

2. INVENTORY AND RADIOACTIVE DECAY

This section describes, at a high level, the waste inventory to be disposed of in the DGR as well as the theory of radioactive decay which will reduce the hazard of the wastes over time and is included into all components of the ISM.

2.1 Used Fuel Inventory

The inventory of used fuel currently in interim storage in Canada consists primarily of 37- element natural uranium CANDU fuel bundles, their variants, as well as a significant quantity of 28-element bundles. Variants include the 37R (regular) bundle, the 37-element long length bundle and the 37M (modified) bundle[1], while additionally there are some older bundles that do not have the CANLUB coating (a thin graphite layer between the fuel pellet and the fuel sheath). Other fuel bundles in storage include small quantities of 7-element bundles, 18-element bundles[2], 19-element[3] bundles, and 43-element CANFLEX LVRF bundles[4].

The inventory of used fuel currently in interim storage in Canada includes also a small quantity of experimental and research reactor fuels developed by Atomic Energy of Canada Limited (AECL) in prior decades. The AECL fuels are diverse in design and composition; however, the quantity is small relative to the inventory of used CANDU fuels.

The projection for the used CANDU fuel bundles at the end of life of the current reactor fleet in Canada, based on the plans for refurbishment and life extension for the current reactor fleet available as of 30 June 2024, was approximately 5.9 million used CANDU equivalent fuel bundles (Reilly, 2024). It is estimated that the inventory of AECL used research fuels currently in interim storage is approximately equivalent to 3,400 37-element CANDU bundles based on the inventory, mass and burnup of the various AECL fuels[5] (Reilly, 2024); this quantity is included in the total number of CANDU equivalent fuel bundles.

Fuel geometries are not explicitly represented in the ISM (see Section 3) and a diverse range of used fuel or other wasteforms can be considered through input parameters defining the fuel.

2.2 Facility Generated Low and Intermediate Level Wastes

In addition to the fuel, low and intermediate level wastes will be generated through operations of the DGR. Following operations, low level wastes are assumed to be disposed of in the DGR and intermediate level wastes are assumed to be shipped to a separate facility for final disposal.

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[1] A modified 37-element bundle (37M) has entered service in some stations; however, the changes are minor relative to a standard 37-element bundle and are not significant to disposal.

[2] A small quantity of 18-element fuel is currently in dry storage after use in the Gentilly 1 CANDU-BLW boiling water reactor prototype.

[3] A small quantity of 19-element fuel is currently in dry storage after use in the Douglas Point and Nuclear Power Demonstration prototype reactors.

[4] A 43-element bundle with a central element composed of Dysprosium has been used in a limited fashion in Bruce B reactors.

[5] This estimate is the mass-based estimate of the number of bundle equivalents in the AECL inventory and includes the majority of the research reactor and experimental fuels in the AECL fuel inventory. The remaining inventory items will be assessed with respect to their suitability for disposal in the APM deep geological repository and have therefore been excluded at this time.

2.3 Contaminant Inventory in the Wasteforms

Inventories of contaminants (radionuclides and stable isotopes) present in the used fuel matrix, cladding (including surface deposits) and facility generated low level wastes are inputs to the ISM.

2.4 Radioactive Decay and Ingrowth

For radionuclides included in the ISM, decay and ingrowth is modelled in each component model of the ISM using the Bateman equation (Bateman, 1910). Decay of a single radionuclide or radionuclide i is described by:

$$-\frac{dN_i}{dt} = \lambda_i N(t) \tag{2-1}$$

The solution to this first-order differential equation is:

$$N_i(t) = N_{i,0} e^{-\lambda_i t} \tag{2-2}$$

where,

$N_i(t)$	is the amount of radionuclide i at time t;
$N_{i,0}$	is the initial amount of a given radionuclide;
λ_i	is the decay rate constant of radionuclide i [1/s]; and
t	is time [s].

In the case where a daughter radionuclide i is generated via decay of a parent radionuclide i-1, the amount of radionuclide i is described by:

$$-\frac{dN_i}{dt} = -\lambda_i N_i(t) + \lambda_{i-1} N_{i-1}(t) \tag{2-3}$$

In the ISM component models, Equation (2-3) is solved numerically by the underlying codes. Branching and rejoining decay chains are allowed. Decay into more than one daughter is handled by the user setting the decay rate to reflect the probability of each decay occurring i.e. the relative probability of A decaying to B or C is not given explicitly but is implicit in the decay rates given for the A-to-B and A-to-C decay processes. There are no limits on the length of a decay chain outside of computation time.

3. WASTEFORM MODEL

3.1 Wasteform Model Overview

The ISM v1.4 introduces a new component, the wasteform model (also referred to as the ISM-WF model). The ISM-WF model estimates radionuclide and element "source terms" from a variety of wasteforms that may be disposed of in the deep geologic repository (DGR) (e.g., CANDU fuels, prototype fuels and research fuels, and DGR facility generated low level wastes).

Compartments are used to represent the fuel (or waste), cladding, and surface deposits. Radionuclides present in these compartments can then be transferred to the "waste package" (e.g., used fuel container) compartment which then transfers contaminants to the geosphere (represented as a sink compartment). The flux of contaminants to the geosphere is the output of the ISM-WF model. Figure 3-1 below summarises the conceptual model of ISM-WF initialization and transfers as implemented in AMBER.

The ISM-WF model assumes that waste packages fail at a user specified time (specified in the model input data) at which point there is sufficient water available to fill the waste package and to provide a pathway connecting the wasteform, cladding and surface deposits to the buffer surrounding the waste package. The ISM-WF model does not model the mechanism of waste package failure (e.g., corrosion).

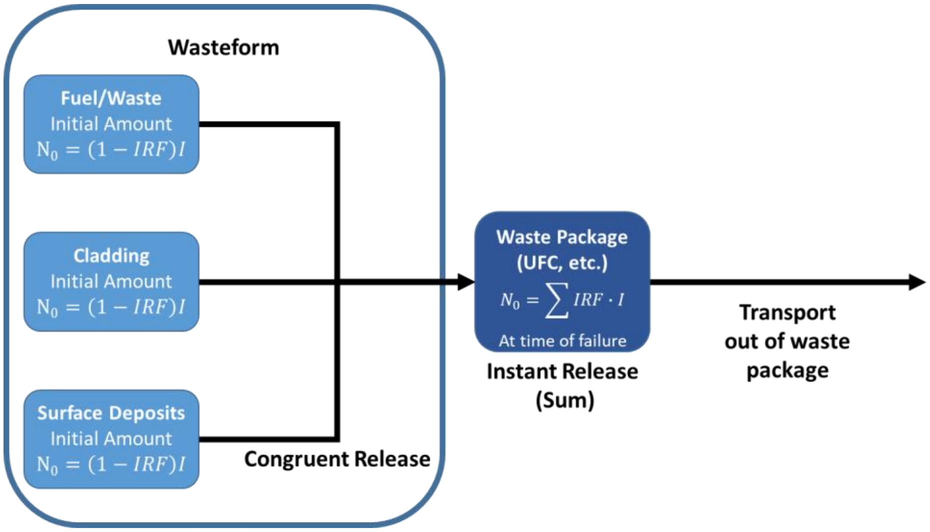

Figure 3-1: ISM-WF Implementation in AMBER

The initial amounts of contaminants in the fuel/waste, cladding and surface deposit compartments are described Section 3.2.1. The instant release of contaminants in the waste package is described in Section 3.2.2. Congruent releases from the fuel/waste, cladding and surface deposits are described in Section 3.2.3. Transport out of the waste package (i.e., interface with the geosphere model) is described in Section 3.2.4.

When the ISM-WF model is used, the ISM-NF becomes an optional component of ISM for use depending on the scenarios being modelled or for verification and validation activities. An overview of the ISM-NF model and associated model theory is described in Appendix A.

3.2 Wasteform Model Theory

The following sections summarize the theory specific to the ISM-WF model.

3.2.1 Initial Amount in the Fuel/Waste, Cladding, and Surface Deposit Compartments

The ISM-WF model is based on the various wasteform configurations that will be disposed of in the DGR (e.g., CANDU fuels, prototype and research fuels, low level wastes). The wasteform conceptualisation includes separate releases from the fuel/waste, cladding, and surface deposits.

In the ISM-WF model the wasteform geometry is not explicitly represented so geometric differences in fuels, wasteforms or cladding are not realized. However, the amounts and surface areas are accounted for in the congruent dissolution models (see Section 3.2.3). Variations in the wasteform type, composition, burnup, and power can be captured via the inventory of contaminants in the wasteform and other model input parameters.

Some radionuclides and stable elements (notably the more volatile contaminants) may be released more rapidly than those in the bulk materials. For example, Figure 3-2 (Johnson et al. 1994) shows how radionuclides and stable elements can be distributed within a used fuel bundle. Therefore, when the waste package is breached and the wasteform, cladding or surface deposits are contacted by water, the location of the nuclides affects the rate at which they are released into the groundwater.

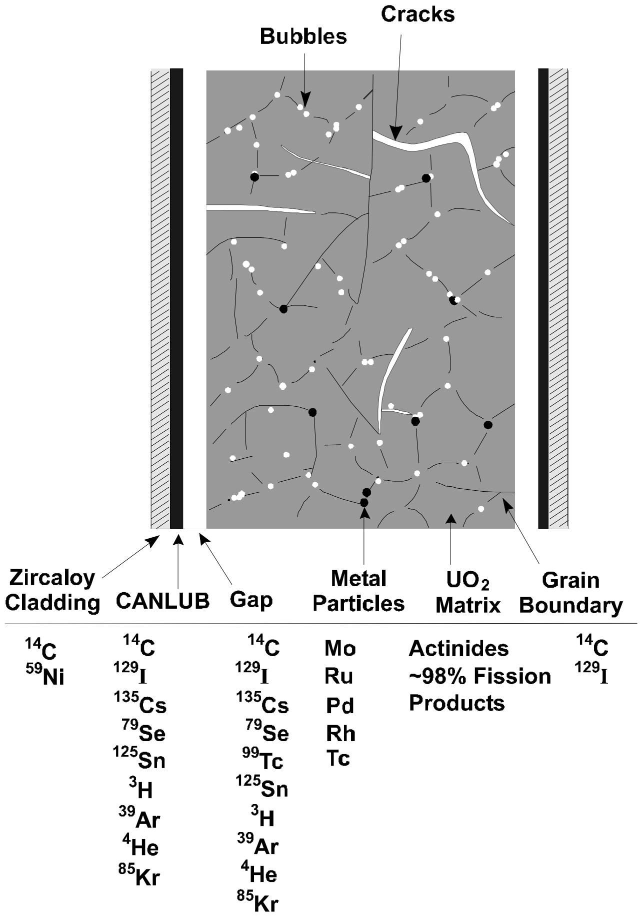

Figure 3-2: Distribution of Various Radionuclides within a Used Fuel Element

Each wasteform component is assumed to have a fraction that will be released instantaneously and the remainder that will be released through slower degradation processes. The amount released by instant release is described in Section 3.2.2, and the slow “congruent” release is described in Section 3.2.3. The initial amount of contaminant in each wasteform component (fuel / waste, cladding and surface deposits), per waste package, considers the instant release fraction has been removed, with the remainder available for congruent release and is given by:

$$\mathrm{N}_{0,w}^{\mathrm{j}} = \mathrm{I}_{\mathrm{w}}^{\mathrm{j}} \cdot \mathrm{M}_{\mathrm{w}}^{\mathrm{j}} \cdot \mathrm{a}_{w} \cdot \mathrm{n}_{w} \cdot (1 - f_{IRF,w}^{j}) \tag{3-1}$$

where,

$\mathrm{N}_{0,w}^{\mathrm{j}}$	is the initial amount of contaminant j in wasteform component w [$\mathrm{kg}_{\mathrm{contaminant}}$] per waste package;
$\mathrm{I}_{\mathrm{w}}^{\mathrm{j}}$	is the inventory of contaminant j in wasteform component w [$\mathrm{mol}_{\mathrm{contaminant}}$ / $\mathrm{kg}_{\mathrm{wasteform\ component}}$];
$\mathrm{M}_{\mathrm{w}}^{\mathrm{j}}$	is the molar mass of contaminant j in wasteform component w [$\mathrm{kg}_{\mathrm{contaminant}}$ / $\mathrm{mol}_{\mathrm{wasteform\ component}}$];
a_{w}	is the amount of wasteform component w per wasteform [$\mathrm{kg}_{\mathrm{wasteform\ component}}$ / wasteform];
n_{w}	is the number of wasteforms per waste package [wasteform]; and
$f_{IRF,w}^{j}$	is the fraction of contaminant j release instantly from the wasteform component w upon contact with water [-].

3.2.2 Instant Release from the Fuel / Waste, Cladding and Surface Deposits

All wasteform components of the ISM-WF model (fuel / waste, cladding and surface deposits) may have a small fraction of the initial inventory released rapidly upon contact with water. This fraction of the radionuclide inventory is referred to as the instant release fraction.

In the ISM-WF model the instant release is implemented as the initial amount in the waste package compartment and includes contributions from all wasteform components. Therefore, the initial amount of contaminant j in the waste package is given by:

$$\mathrm{N}_{0,wp}^{\mathrm{j}} = \sum_{w} \left[\mathrm{I}_{\mathrm{w}}^{\mathrm{j}} \cdot \mathrm{M}_{\mathrm{w}}^{\mathrm{j}} \cdot \mathrm{a}_{w} \cdot \mathrm{n}_{w} \cdot f_{IRF,w}^{j}\right] \tag{3-2}$$

where,

$\mathrm{N}_{0,wp}^{\mathrm{j}}$	is the initial amount of contaminant j in the waste package [$\mathrm{kg}_{\mathrm{contaminant}}$];
$\mathrm{I}_{\mathrm{w}}^{\mathrm{j}}$	is the inventory of contaminant j in wasteform component w [$\mathrm{mol}_{\mathrm{contaminant}}$ / $\mathrm{kg}_{\mathrm{wasteform\ component}}$];
$\mathrm{M}_{\mathrm{w}}^{\mathrm{j}}$	is the molar mass of contaminant j in wasteform component w [$\mathrm{kg}_{\mathrm{contaminant}}$ / $\mathrm{mol}_{\mathrm{wasteform\ component}}$];
a_{w}	is the amount of wasteform component w per wasteform [$\mathrm{kg}_{\mathrm{wasteform\ component}}$ / wasteform];
n_{w}	is the number of wasteform per waste package [wasteform]; and
$f_{IRF,w}^{j}$	is the fraction of contaminant j release instantly from the wasteform w upon contact with water [-].

Note that no transfer from the waste components to the waste package or out of the waste package can occur until the package is failed (timing specified via user input). Prior to failure decay and ingrowth of the radionuclides in the waste component and waste package compartments occurs.

3.2.3 Congruent Release from the Fuel/Waste, Cladding, and Surface Deposit Compartment

The contaminants in the fuel/waste, cladding and surface deposits, may dissolve slowly in water due to various mechanisms. The ISM-WF explicitly includes the following congruent release mechanisms:

1. Linear (fractional) release rate.
2. Weighted fractional release rate. Similar to above (1) with a linear, user defined and time-dependent weighting.
3. Radiolytic dissolution rate.
4. One dimensional corrosion rate.
5. User defined time dependent release rate.

3.2.3.1 Linear Fractional Release Rate

For the linear (fractional) release rate, the congruent degradation rate is fixed and a set fraction (e.g., 10^{-7}/a) of the wasteform component (fuel / waste, cladding, surface deposits) is transferred from the wasteform component compartment to the waste package compartment. Consequently, the fractional release rate of contaminant j entering the waste package at time t is given by:

$$F_{linear}^{j}(t) = \delta_t^{fail} \cdot \mathrm{N}_w^j(\mathrm{t}) \cdot C_{linear,w}/(1 - C_{linear,w} \cdot (\mathrm{t} - t_{fail})) \tag{3-3}$$

where,

$F_{linear}^{j}(t)$	is fractional release rate of contaminant j entering the waste package at time t [$\mathrm{kg}_{\mathrm{contaminant}}$/a];
$N_w^j(\mathrm{t})$	is the amount of contaminant j in the wasteform w as determined by the wasteform model [$\mathrm{kg}_{\mathrm{contaminant}}$];
$C_{linear,w}$	is the linear fractional degradation rate of the wasteform component w [1/a];
δ_t^{fail}	is a Boolean parameter that is 1 if $t < t_{fail}$ and 0 if $t > t_{fail}$ [-];
t	is the time [a]; and
t_{fail}	is time of waste package failure [a].

3.2.3.2 Weighted Fractional Release Rate

The weighted fractional release is similar to the linear fractional release rate. However, the congruent degradation rate is now weighted to decrease with time. This is implemented in the ISM-WF model by applying a linearly decreasing weighting factor to the linear fractional degradation rate.

For example, given a weighting factor of 10% the initial fractional degradation would be increased by factor 1.1 then reduced linearly over the total congruent degradation rate timeframe (e.g., 10 million years for a linear fraction degradation rate of 10^{-7}/a) to a factor of 0.9.

A physical example of weighted release mechanism of this type is time varying surface areas which could reduce from the post-irradiation areas to smaller areas as the fuel dissolves. The larger initial fuel surface areas could result in a higher initial congruent degradation rate that will decrease with time.

The weighted fractional release rate of contaminant j entering the waste package is given by:

$$F^{j}_{weighted}(t) = \delta^{fail}_{t} \cdot \mathrm{N}^{\mathrm{j}}_{w}(\mathrm{t}) \cdot W(t) \cdot \frac{a_w \cdot n_w}{A(t)} \tag{3-4}$$

where,

$F^{j}_{weighted}$	is weighted fractional release rate of contaminant j entering the waste package at time t [$\mathrm{kg}_{\mathrm{contaminant}}$/a];
$A(t)$	is the analytical expression for the remaining species amount as defined by Equation (3-5);
$W(t)$	is the time dependent weighting function [-] as defined by Equation (3-7);
$N^{j}_{w}(\mathrm{t})$	is the amount of contaminant j in the wasteform w as determined by the wasteform model [$\mathrm{kg}_{\mathrm{contaminant}}$];
a_w	is the amount of wasteform component w per wasteform [$\mathrm{kg}_{\mathrm{wasteform\ component}}$ / wasteform];
n_w	is the number of wasteforms per waste package [wasteform]; and
δ^{fail}_{t}	is a Boolean parameter that is 1 if $t < t_{fail}$ and 0 if $t > t_{fail}$ [-].

The analytical expression $A_f(t)$ representing the remaining species amount is of the form:

$$A(t) = \frac{1}{2} \cdot a \cdot t^2 - b \cdot t + c \tag{3-5}$$

where,

$$\begin{aligned} a &= -2\mathrm{N}^{j}_{0,w} \cdot w \cdot \left(C_{linear,w}\right)^2 - 1 \\ b &= -\mathrm{N}^{j}_{0,w} \cdot C_{linear,w}\left[1 + w \cdot \left(1 + 2C_{linear,w} \cdot t_{fail}\right)\right] \\ c &= \mathrm{N}^{j}_{0,w} - \frac{1}{2}\left(a \cdot {t_{fail}}^2\right) - b \cdot t_{fail} \end{aligned} \tag{3-6}$$

where,

$\mathrm{N}^{j}_{0,w}$	is the initial amount of contaminant j in wasteform component w [$\mathrm{kg}_{\mathrm{contaminant}}$];
w	is the weighting factor [-];
$C_{linear,w}$	is the linear fraction degradation rate of the wasteform component w [1/a]; and
t_{fail}	is time of waste package failure [a].

The time dependent weighting function, $F_w(t)$, is defined using the AMBER *rampDown* function which linearly interpolates from one to zero between time steps, t_{fail} and $1/C_{linear,w}$. The time dependent weight function is given by Equation (3-7) and is illustrated in Figure 3-3.

$$W(t) = 1 + \left[\left(rampDown_{1/C_{linear,w}}^{t_{fail}} \cdot 2w\right) - \mathrm{w}\right] \tag{3-7}$$

where,

w	is the weighting factor (-); and
t_{fail}	is time of waste package failure [a].

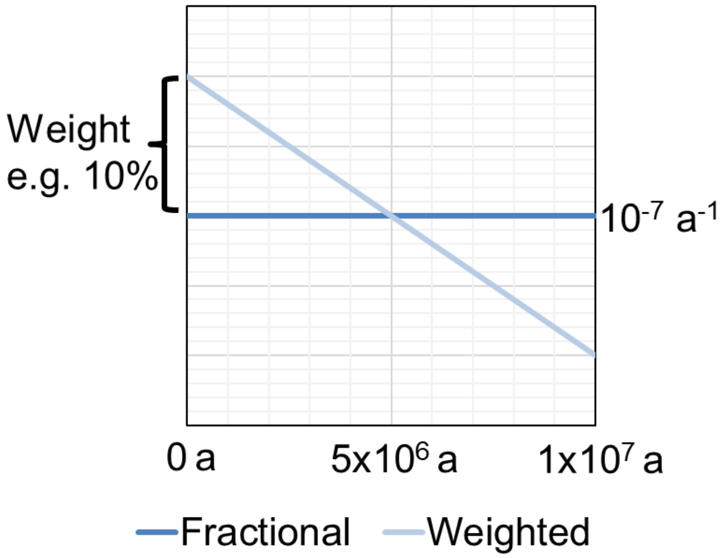

Figure 3-3: Illustration of Release Rate: Fractional vs Weighted Release Rate

3.2.3.3 Radiolytic Dissolution Rate

The radiolytic dissolution rate release only applies to the fuel component of the wasteform and is given by Equation (3-8) which follows the same general form as Equation (3-3)[6].

$$F_{radiolytic}^{j}(t) = \delta_t^{fail} \cdot \mathrm{N}_w^j(\mathrm{t}) \cdot \frac{C_{rad,fuel}(t)}{a_{fuel} \cdot n_{fuel} \cdot I_{fuel}^{UO2}} / (1 - \frac{C_{rad,fuel}(t)}{a_{fuel} \cdot n_{fuel} \cdot I_{fuel}^{UO2}} \cdot (\mathrm{t} - t_{fail})) \tag{3-8}$$

where,

$F_{radiolytic}^{j}(t)$	is radiolytic release rate of contaminant j entering the waste package at time t [$kg_{contaminant}$/a];
$N_w^j(\mathrm{t})$	is the amount of contaminant j in the fuel as determined by the wasteform model [$kg_{contaminant}$];
a_{fuel}	is the amount of fuel per wasteform (e.g., bundle) [kg_{fuel} / wasteform];
n_{fuel}	is the number of wasteforms (e.g., fuel bundles) per waste package [wasteform];
$\mathrm{I}_{\mathrm{fuel}}^{U02}$	is the initial inventory of UO_2 in wasteform component w [mol_{UO2} / $kg_{wasteform\ component}$];

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[6] Equation (3-3) assumes the congruent release rate is not time dependant. The radiolytic dissolution rate is time dependant, the effect of applying the general form of Equation (3-3) for radiolytic dissolution is shown in Section 3.2.3.3.

δ_t^{fail}	is a Boolean parameter that is 1 if $t < t_{fail}$ and 0 if $t > t_{fail}$ [-];
t_{fail}	is time of waste package failure [a]; and
$C_{rad,fuel}(t)$	is the radiolytic matrix degradation rate of wasteform w, at time t [mol/a] given by Equation (3-9).

$$C_{rad,fuel}(\mathrm{t}) = A_{fuel}\left[G_\alpha f_\alpha D_\alpha(t)^{a\alpha} + G_\beta f_\beta D_\beta(t)^{a\beta} + G_\gamma f_\gamma D_\gamma(t)^{a\gamma} + R_{Uchem}\right] \tag{3-9}$$

where,

A_{fuel}	is the effective surface area of the fuel [m^2];
$D_\alpha(t)$	is the time-dependent alpha dose rates [Gy/a];
$D_\beta(t)$	is the time-dependent beta dose rates [Gy/a];
$D_\gamma(t)$	is the time-dependent gamma dose rates [Gy/a];
G_α, G_β, G_γ	are empirical rate constants for fuel dissolution in the presence of alpha, beta and gamma radiation fields, respectively [$\mathrm{mol_{UO2}/m^2/Gy}$];
f_α, f_β, f_γ	are the alpha dose, beta dose, and gamma dose variability factors, accounting for uncertainties in the radiation field strengths due to, for example, uncertainties in the contaminant inventories, and are approximately equal to unity [-];
$a\alpha$, $a\beta$, $a\gamma$	are fitting parameters for the dependence of the fuel dissolution rate on the alpha, beta, and gamma dose rates, and are approximately equal to one [-]; and
R_{Uchem}	is the chemical fuel dissolution rate, i.e., the dissolution rate of the fuel in the absence of radiolysis [$\mathrm{mol_{UO2}/m^2/a}$].

3.2.3.4 One Dimensional Corrosion Rate

The one-dimensional corrosion release rate is given by Equation (3-10) and follows the same general form as Equation (3-3).

$$F^j_{corrosion}(t) = \delta_t^{fail} \cdot \delta_t^{max} \cdot \mathrm{N}_w^j(\mathrm{t}) \frac{C_{cor,w}}{(\mathrm{d}_{c,w} - C_{cor,w} \cdot (\mathrm{t} - t_{fail}))} \tag{3-10}$$

where,

$F^j_{corrosion}(t)$	is 1-D corrosion release rate of contaminant j entering the waste package at time t [$\mathrm{kg_{contaminant}/a}$];
$N_w^j(\mathrm{t})$	is the amount of contaminant j in the wasteform w as determined by the wasteform model [$\mathrm{kg_{contaminant}}$];
$C_{cor,w}$	is the corrosion rate of the wasteform component w [$\mathrm{m_{wasteform}}$ / a];
$\mathrm{d}_{c,w}$	is the thickness or characteristic depth of wasteform component w [$\mathrm{m_{wasteform}}$];
δ_t^{fail}	is a Boolean parameter that is 1 if $t < t_{fail}$ and 0 if $t > t_{fail}$ [-];
δ_t^{max}	is a Boolean parameter that is 1 if $t < t^{max}_{corrosion}$ given by Equation (3-11) and 0 if $t > t^{max}_{corrosion}$ [-]; and
t_{fail}	is time of waste package failure [a].

where

$$t^{max}_{corrosion} = d_{c,w}/C_{cor,w} \tag{3-11}$$

3.2.3.5 User Defined Time Dependent Release Rate

The user defined time dependent release rate is given by:

$$F_{UD}^{j}(t) = \delta_{t}^{fail} \cdot \mathrm{N}_{w}^{j}(\mathrm{t}) \cdot C_{user,w}(t) \tag{3-12}$$

where,

$F_{UD}^{j}(t)$	is user defined release rate of contaminant j entering the waste package at time t [$\mathrm{kg_{contaminant}}$/a];
$N_{w}^{j}(\mathrm{t})$	is the amount of contaminant j in the wasteform w as determined by the wasteform model [$\mathrm{kg_{contaminant}}$];
$C_{user,w}(t)$	is the time dependent user defined release rate of the wasteform component w at time t [1/a];

3.2.4 Transport Out of the Waste Package (Interface with the Geosphere Model)

Transport out of the waste package is controlled by flow and diffusion in saturated porous media and the solubility limit of a given contaminant.

In an advective environment, the rate of contaminant j leaving the waste package is defined by the flow rate through the package. The flow rate through the package is an input to the model and will depend on the specific advective case being considered. In general, with sufficiently high advective velocities the release from the waste package will be limited by the congruent dissolution rate of the wasteform components (fuel / waste, cladding, and surface deposits).

In a diffusion dominant regime, the transport of contaminants is defined by diffusion, or Fick's Law (Crank, 1975). Diffusion depends on the system geometry and the ISM-WF model assumes three-dimension spherical shell diffusion for release from the waste package[7].

Solubility limits of contaminants are a property of the underlying chemical element. They may limit the transfer rate out of a waste package. For example, both U-234 and U-238 contribute to the same solubility of uranium and the concentration of uranium in solution in the waste package will not exceed the solubility limit. In ISM-WF the shared limit scheme (Section 9.14.3 of Quintessa 2023) is used to implement solubility limits.

Therefore, the transfer from the waste package to the geosphere is given by:

$$X_{wp}^{j}(t) = \delta_{t}^{fail} \cdot Sol^{j}(t) \cdot \frac{N_{wp}^{j}(\mathrm{t})}{V_{wp}} \cdot \left[Q(t) + \ 4\pi D_{eff}^{j}\left(\frac{r_1 r_2}{r_2 - r_1}\right)\right] \tag{3-13}$$

where,

$X_{wp}^{j}(t)$	is the rate of contaminant j leaving the waste package [kg/a];
δ_{t}^{fail}	is a Boolean parameter that is 1 if $t < t_{fail}$ and 0 if $t > t_{fail}$ [-];
V_{wp}	is the volume of the waste package [$\mathrm{m^3}$];
$\mathrm{Q(t)}$	is the infiltration rate through the waste package volume in an advective environment [$\mathrm{m^3/a}$];

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[7] Note a 3D spherical shell diffusion is conservative, with a greater mass flux relative to a two-dimensional cylindrical shell geometries or a one-dimensional diffusion.

$N_{wp}^{j}(t)$	is the amount of contaminant j in the waste package at time t [kg];
D_{eff}^{j}	is the effective diffusion coefficient of contaminant j in the buffer [m^2/a];
$Sol^{j}(t)$	is the fraction released of contaminant j at time t as limited by the elemental solubility limit [-] and is given by Equation (3-16); and
r_2	is radius of the effective buffer thickness [m] given by Equation (3-14).

$$r_2 = r_1 + t_b \tag{3-14}$$

where,

t_b	is the minimum thickness of the buffer [m_{buffer}];
r_1	is radius of the waste package effective sphere geometry [m] given by Equation (3-15):

$$r_1 = \sqrt{A_{wp}/4\pi} \tag{3-15}$$

where,

A_{wp}	is the area of the waste package [m^2]

The solubility limit depends on the element concentrations and is given by:

$$Sol^{j}(\mathrm{t}) = \min\left(\frac{Sol_{lim}^{i} V_{wp}}{\sum_{j}^{i} N_{wp}^{j}(t)}, 1\right) \tag{3-16}$$

where,

$Sol^{j}(t)$	is the fraction released of contaminant j at time t as limited by the elemental solubility limit [-]
Sol_{Lim}^{i}	is the solubility limit of element i [kg/m^3];
V_{wp}	is the volume of the waste package [m^3]; and
$\sum_{j}^{i} N_{wp}^{j}(t)$	is the sum of the amounts of all contaminant isotopes j of a given element i in the waste package at time (t) [kg];

4. GEOSPHERE MODEL

4.1 Geosphere Model Overview

The geosphere model (also referred to as the ISM-GEO model) is the finite element model representing the flow and contaminants transport through the geosphere and is developed using HydroGeoSphere (HGS) (Aquanty 2015). The geosphere model representing the Revell Site includes a simplified representation of the repository, the host rock, any significant geosphere features (e.g., fractures, faults, and aquifers) present at the repository site as well as known water wells. Site characterization boreholes will be sealed prior to closure of the repository.

In general, the geosphere model determines the steady-state groundwater flow field and the subsequent transport of contaminants from the repository to the surface environment. Transient groundwater flow fields (e.g., resulting from advancing and retreating of glaciers) may be considered in future versions of the ISM-GEO model.

The general theory applicable to the geosphere model includes:

- Complete hydrologic modelling of the subsurface flow consisting of 3D saturated flow.
- Arbitrary combinations of porous, discretely-fractured, dual-porosity and dual-permeability media for the subsurface.
- Accurate handling of fluid and mass exchanges between fractures and matrix including matrix diffusion effects and solute advection in the matrix.
- Automatic and correct apportioning of the total flow rate of a multi-layer well to the well nodes, including the simulation of water flow and solute mixing within the water column in the well.
- Straight or branching decay chains representing degradation reactions.

Section 4.2 describes relevant components of the HGS theory applicable to the current ISM-GEO model. A detailed description of the complete HGS theory (including features not used by the ISM-GEO model) as well as the numerical implementation of said theory is given in Aquanty (2015).

4.2 General Geosphere Model Theory

The following sections summarize the groundwater flow and contaminant transport theory specific to the ISM-GEO model.

4.2.1 Subsurface Flow in Saturated Porous Media

Subsurface flow describes the movement of groundwater through the geosphere. In the ISM-GEO models the geosphere system is modelled as saturated porous media. The following assumptions are made for subsurface flow:

- The fluid is incompressible;
- The porous medium and fractures (or macropores), if present, are non-deformable; and
- The system is under isothermal conditions.

Equation (4-1) is a modified form of Richards’ equation (Richards (1931), Equation 2-1 in Aquanty (2015)) used to describe three-dimensional transient subsurface flow in a saturated porous medium in HGS:

$$-\nabla \cdot (w_m q) + \sum \mathit{\Gamma}_{ex} \pm \mathrm{Q} = w_m \frac{\partial}{\partial t}(\theta_m S_w) \tag{4-1}$$

where,

w_m	is the volumetric fraction of the total porosity occupied by the porous medium (or primary continuum). This volumetric fraction is always equal to 1.0 except when a second porous continuum is considered for a simulation, which is the case when the dual continuum option is used to represent existing fractures or macropores.
q	is the fluid flux [m/s], given by Equation (4-2) (Equation 2.2 in Aquanty (2015)).
$\mathit{\Gamma}_{ex}$	is the volumetric fluid exchange rate [m^3/m^3/s] between the subsurface domain and all other types of domains supported by the model and it is expressed per unit volume of the other domain types. Currently, these additional domains are surface, wells, tile drains, discrete fractures and dual continuum.
Q	is fluid exchange with the outside of the simulation domain, as specified from boundary conditions [m^3/m^3/s], which is a volumetric fluid flux per unit volume representing a source (positive) or a sink (negative) to the porous medium system.
θ_m	is the porosity of the medium [-]; and
S_w	is the water saturation [-], assumed to be 1 or fully saturated.

$$\mathrm{q} = -\mathrm{K} \cdot k_r \nabla(\psi + z) \tag{4-2}$$

where,

k_r	represents the relative permeability of the medium [-];
ψ	is the pressure head [m];
z	is the elevation head [m]; and
K	is the hydraulic conductivity tensor [m/s] and is given by Equation (4-3) (Equation 2.3 in Aquanty (2015))

$$\mathrm{K} = \frac{\rho g}{\mu} \mathrm{k} \tag{4-3}$$

where,

g	is the gravitational acceleration [m/s^2];
ρ	is the density of water [kg/m^3];
μ	is the viscosity of water [kg/m/s]; and
k	is the permeability tensor of the permeable media [m^2].

4.2.2 Subsurface Flow in Discrete Fractures

HGS is capable of modelling discrete fractures and porous media in a dual continuum based on the formulation presented by Gerke and Genuchten (1993). In the dual continuum approach the porous medium is linked to a discrete feature such as a fracture via the fluid flux defined in Equation (4-2).

Fractures in HGS are idealized as the space between two parallel surfaces, with the tacit assumptions that the total head is uniform across the fracture width. The equation for saturated flow in a fracture is based on Berkowitz et al. (1988) and Sudicky and Mclaren (1992) and is given by the two-dimension saturated flow Equation (4-4) (Equation 2.11 in Aquanty (2015)).

This is analogous to the Richards Equation for porous media (Equation (4-1)). Note that channelling is not considered in the ISM-GEO models at this time.

$$-\overline{\overline{\nabla}} \cdot \left(w_f q_f\right) + w_f \Gamma_f = w_f \frac{\partial}{\partial t}\left(S_{wf}\right) \tag{4-4}$$

where,

w_f	is the fracture width [m]
q_f	is the fracture fluid flux [m/s], given by Equation (4-5) (Equation 2.12 in Aquanty (2015));
Γ_f	is the fluid exchange rate [m^3/m^3/s] between the subsurface domain and fracture; and
S_{wf}	is the water saturation in the fracture [-], assumed to be 1 or fully saturated.

$$q_f = -\mathrm{K}_f \cdot k_{rf} \overline{\overline{\nabla}}\left(\psi_f + z_f\right) \tag{4-5}$$

where,

k_{rf}	represents the relative permeability of the fracture [-];
ψ_f	is the pressure head in the fracture [m];
z_f	is the elevation head in the fracture [m]; and
K_f	is the hydraulic conductivity tensor [m/s] and is given by Equation (4-6) (Equation 2.13 in Aquanty (2015)).

$$\mathrm{K}_f = \frac{\rho g w_f}{12\mu} \tag{4-6}$$

where,

g	is the gravitational acceleration [m/s^2];
ρ	is the density of water [kg/m^3];
μ	is the viscosity of water [kg/m/s]; and
w_f	is the fracture width [m].

4.2.3 Subsurface Flow in the Well

Groundwater wells are assumed in the geosphere models in most simulations. They are used to provide water for domestic use by various receptors living on the surface near the repository site. In general, the length of the well will be much larger than the cross-sectional area of the well casing. Consequently, well hydraulic properties and fluid flow can be simplified, integrated, and averaged over the well cross-section into a one-dimensional approximation.

Saturated groundwater flow along the axis of a well, assuming laminar conditions is described by Equation (4-7), (4-8) and (4-9) (Section 2.3.2.2 of Aquanty (2015), specifically Equations 2.60 and 2.61).

$$Q_{1D} = -\left(\pi r_w^2\right)\left(\frac{r_w^2 \rho g}{8\mu}\right)\frac{\partial h_w(s)}{\partial s} \tag{4-7}$$

$$\frac{\partial}{\partial s}\left(\pi r_w^4 \frac{\rho g}{8\mu}\frac{\partial h_w(s)}{\partial s}\right) + Q_w \delta\left(s - s_p\right) + \Gamma_{pm \to w} = \pi r_w^2 S_{sw} \frac{\partial h_w(s)}{\partial t} \tag{4-8}$$

$$S_{sw} = \rho g \beta \tag{4-9}$$

where,

Q_{1D}	is the fluid flux along the one-dimensional well axis [m^3/s]. This parameter is Q_{well}^{l} in the biosphere model (Equation (5-1));
r_w	is the well radius [m];
ρ	is the density of water in [kg/m^3];
g	is the gravitational acceleration [m/s^2];
μ	is the viscosity of water [kg/m/s];
$h_w(s)$	is the well hydraulic head at position s along the well axis [m];
s	is the well coordinate along the well axis [-];
Q_w	is the well discharge (or recharge) per unit length [m^2/s];
$\Gamma_{pm\rightarrow w}$	is the fluid exchange between the surrounding porous medium (pm) and the well (w) [m^2/s]. $\Gamma_{pm\rightarrow w}$ is defined by Equation (4-10) assuming a flux continuity between the well and surrounding medium (Equation 2.64 in Aquanty (2015));
S_{sw}	is the specific storage coefficient for a fluid filled borehole [1/m]; and
β	is the compressibility of water [m·s^2/kg].

$$\Gamma_{pm\rightarrow w} = -2\pi r_w (k_r)_{exch(pm,w)} K_{exch(pw,w)} \frac{h_w(s) - h}{l_{exch(pm,w)}} \tag{4-10}$$

where,

$(k_r)_{exch(pm,w)}$	is the upstream relative permeability [-], equal to $(k_r)_{pm}$ if $h \geq h_w(s)$ and $(k_r)_w$ if $h < h_w(s)$;
$K_{exch(pw,w)}$	is the hydraulic conductivity of the exchange thickness defining the interface between the porous media and the well [m/s];
$l_{exch(pm,w)}$	is the exchange thickness defining the interface between the porous media and the well [m]; and
h	is the hydraulic head in the porous media [m].

4.2.4 Transport in Saturated Porous Media

Three-dimensional transport of solutes in a saturated porous media is described by Equation (4-11) (Equation 2.116 in Aquanty (2015)):

$$\begin{aligned} -\nabla \cdot w_m\left(qC_j - \theta_m S_w D \nabla C_j\right) + w_m \theta_m S_w R_{j-1} \lambda_{j-1} C_{j-1} + \sum \Omega_{ex} \pm Q_c \\ = w_m \left(\frac{\partial\left(\theta_m S_w R_j C_j\right)}{\partial t} + \theta_m S_w R_j \lambda_j C_j \right) \end{aligned} \tag{4-11}$$

where,

w_m	is the volumetric fraction of the total porosity occupied by the porous medium (or primary continuum). This volumetric fraction is always equal to 1.0 except when a second porous continuum is considered for a simulation, which is the case when the dual continuum option is used to represent existing fractures or macropores.
q	is the fluid flux [m/s] given by Equation (4-2);
C_j	is the solute concentration [kg/m^3] of contaminant j;
θ_m	is the porosity of the medium [-];

S_w	is the water saturation [-], assumed to be 1 or fully saturated;
D	is the hydrodynamic dispersion tensor [m^2/s] given by Equation (4-13). Originally from Bear (1972) and is Equation 2.118 in Aquanty (2015);
λ_j	is a first-order decay constant [1/s] of contaminant j. The subscript "j-1" designates parent contaminant for the case of a decay chain;
Ω_{ex}	represents the mass exchange rate of solutes per unit volume [kg/m^3/s] between the subsurface domain and all other types of domains supported by the model (e.g., discrete fractures, wells);
Q_c	represents solute exchange from boundary conditions [kg/m^3/s]; Q_c may represent a source (positive) or a sink (negative) to the porous medium system; and
R_j	represents a dimensionless retardation factor [-] of contaminant j and is given by Equation (4-12). Originally from Freeze and Cherry (1979) and is Equation 2.117 in Aquanty (2015).

$$R_j = 1 + \frac{\rho_b}{\theta_m S_w} Kd_j \tag{4-12}$$

where,

ρ_b	is the bulk density of the porous medium [kg/m^3]; and
Kd_j	is the linear equilibrium sorption coefficient [m^3/kg] of contaminant j.

$$\theta_m S_w D = (\alpha_l - \alpha_t)\frac{qq}{|q|} + \alpha_t |q| I + \theta_s S_w \tau D_{fw}^{j} I \tag{4-13}$$

where,

α_l and α_t	are the longitudinal and transverse dispersivities [m], respectively;
$\lvert q \rvert$	is the magnitude of the fluid flux [m/s];
τ	is the matrix tortuosity [-];
D_{fw}^{j}	is the free-solution diffusion coefficient of contaminant j [m^2/s]; and
I	is the identity tensor [-].

4.2.5 Transport in Discrete Fractures

The equation for two-dimensional solute transport in a fracture is based on Tang et al. (1981), Sudicky and McLaren (1992), Therrien and Sudicky (1996) and is given by Equation (4-14) (Equation 2.120 in Aquanty (2015)).

$$\begin{aligned} -\nabla \cdot \left(w_f q_f C_{f,j} - w_f S_{w,f} \mathrm{D}_f \nabla C_{f,j}\right) + w_f R_{f,j-1} \lambda_{j-1} C_{f,j-1} - w_f \Omega_f \\ = w_f \left(\frac{\partial S_{w,f} R_{f,j} C_{f,j}}{\partial t} + S_{w,f} R_{f,j} \lambda_j C_{f,j}\right) \end{aligned} \tag{4-14}$$

where,

w_f	is the fracture width [m].
q_f	is the fluid flux in the fracture [m/s] given by Equation (4-2);
$C_{f,j}$	is the solute concentration [kg/m^3] of contaminant j in the fracture;
$S_{w,f}$	is the water saturation in the fracture [-], assumed to be 1 or fully saturated;

D_f	is the hydrodynamic dispersion tensor [m^2/s] in the fracture given by Equation (4-16). Based on Equation (4-13) (Equation 2.118 in Aquanty (2015)) and assuming the fraction has a porosity of unity;
λ_j	is a first-order decay constant [1/s] of contaminant j. The subscript “j-1” designates parent contaminant for the case of a decay chain;
Ω_f	represents the mass exchange rate of solutes per unit volume [kg/m^3/s] between the fracture and the subsurface domain;
$R_{f,j}$	represents a dimensionless retardation factor [-] of contaminant j and is given by Equation (4-12). Originally from Freeze and Cherry (1979) and is Equation 2.121 in Aquanty (2015).

$$R_{f,j} = 1 + \frac{2K_{f,j}}{w_f} \tag{4-15}$$

where,

$K_{f,j}$	is the fracture-surface distribution coefficient [m] of contaminant j. This is defined as the ratio between the mass of contaminant in the solid phase per unit area of an assumed planar fracture surface area over the concentration of a contaminant in solution.

$$S_{w,f} D_f = \left(\alpha_{l,f} - \alpha_{t,f}\right)\frac{q_f q_f}{\left|q_f\right|} + \alpha_{t,f}\left|q_f\right| I + S_w D_{fw,f}^{j} I \tag{4-16}$$

where,

$\alpha_{l,f}$ and $\alpha_{t,f}$	are the longitudinal and transverse dispersivities [m], respectively;
$\left\lvert q_f \right\rvert$	is the magnitude of the Darcy flux [m/s];
$D_{fw,f}^{j}$	is the free-solution diffusion coefficient of contaminant j [m^2/s]; and
I	is the identity tensor [-].

4.2.6 Transport in the Well

One-dimensional solute transport along the axis of a well is described by Equation (4-17) (Equation 2.127 in Aquanty (2015)):

$$\begin{aligned} -\overline{\nabla}\cdot \pi r_s^2\left(q_w C_{w,j} - S_{ww} D_w^j \overline{\nabla} C_{w,j}\right) + \pi r_s^2 \lambda_{j-1} C_{w,j-1} - \pi r_s^2 \lambda_j C_{w,j} \\ - Q_w\left(C_{w,j} - C_{w,inj,j}\right)\delta(l - l') - \pi r_s^2 \Omega_w = \pi r_s^2 \frac{\partial C_{w,j}}{\partial t} \end{aligned} \tag{4-17}$$

where,

r_s	is the radius of the well [m];
q_w	is the fluid flux along the well axis [m/s];
$C_{w,j}$	is the solute concentration in the well [kg/m^3];
S_{ww}	is the water saturation in the well [-], assumed to be 1 or fully saturated in ISM-GEO;
D_w^j	is the dispersion coefficient in the well given by Equation (4-18);
λ_j	is a first-order decay constant [1/s]. The subscript “j-1” designates parent contaminant for the case of a decay chain;
Q_w	is the well discharge (or recharge) per unit length [m^2/s] applied at location l';
$C_{w,inj,j}$	is the concentration of contaminant j in injected water [kg/m^3];

$\delta(l - l')$	represents a Dirac-delta function, l is the well length along the axis [m], l' is the location at which the well discharges [m]; and
Ω_w	represents the mass exchange rate of solutes per unit volume [kg/m^3/s] between the subsurface domain and the well.

The dispersion coefficient for the well, D_w^j [m^2/s] is originally from Lacombe et al. (1995) and is given by Equation (4-18) (Equation 2.128 in Aquanty (2015)):

$$D_w^j = \frac{{r_s}^2 {q_w}^2}{48 D_{fw}^j} + D_{fw}^j \tag{4-18}$$

where,

r_s	is the radius of the well [m];
q_w	is the fluid flux along the well axis [m/s];
D_{fw}^j	is the free-solution diffusion coefficient of contaminant j [m^2/s].

4.3 Revell Site Geosphere Model

The ISM-GEO model is a detailed transport model that is intended to assess the impact of repository features on flow and transport at the Revell Site. The model is constructed at a higher resolution than the other regional flow models of the area and includes a representation of the repository components (e.g., shafts, access tunnels, placement rooms).

4.3.1 Model Description

Figure 4-1 shows the surface bedrock map of the Revell area (NWMO 2023). The ISM-GEO model domain is a 10 km × 10 km rectangle roughly centred in the blue oval shown in Figure 4-1.

The ISM-GEO model is a dual continuum model in which the intact rock mass is represented by an equivalent porous medium and fractures are represented as a discrete fracture network.

Based on the results of borehole drilling, the intact rock at the Revell site is subdivided into three unique integrated rock units (IRU). The rock units IRU1a and IRU1b show consistent characteristics and the dominant bedrock is biotite granodiorite-tonalite. Rock unit IRU2 consists of predominantly biotite tonalite. Rock unit IRU3 comprises very similar characteristics to the other rock units but includes an increased presence throughout of narrow amphibolites on a sub-metre to metre scale. Figure 4-2 illustrates the spatial distribution of the integrated rock unit domains incorporated in the ISM-GEO model (DesRoches et al. 2021).

Most relevant to the post-closure safety assessment are the higher conductivity features implemented within the models. These include the integrated fracture zone (IFZ), Site Specific Discrete Fracture Network (SSDFN), and higher conductivity planar features associated with the interface between different integrated rock units (IRU). The IFZ fracture set describe large fracture features inferred from surface lineaments with a minimum length of 500 m. The SSDFN consists of a statistically generated random fracture field. This fracture set represents smaller fractures (radius 50 m to 250 m) that are assumed to be embedded in the rock matrix. Fractures are modelled as circles with orientation (dip / strike) conditioned on borehole fracture data. Site characterization data has indicated the presence of large scale sub-horizontal enhanced permeability zones associated with the rock unit transitions. These features are illustrated in Figure 4-3.

Within the ISM-GEO model the repository (e.g., shafts, access tunnels, placement rooms) are represented in sufficient detail (e.g., excavation damaged zone, engineered sealing materials) such that flow and transport through or along the repository components can be resolved. For example, Figure 4-4 illustrates the materials and level of vertical discretization of a placement room included in the ISM-GEO model.

As more site-specific data becomes available and as conceptual designs are refined the ISM-GEO model will continue to be iterated to reflect the latest understanding of the site.

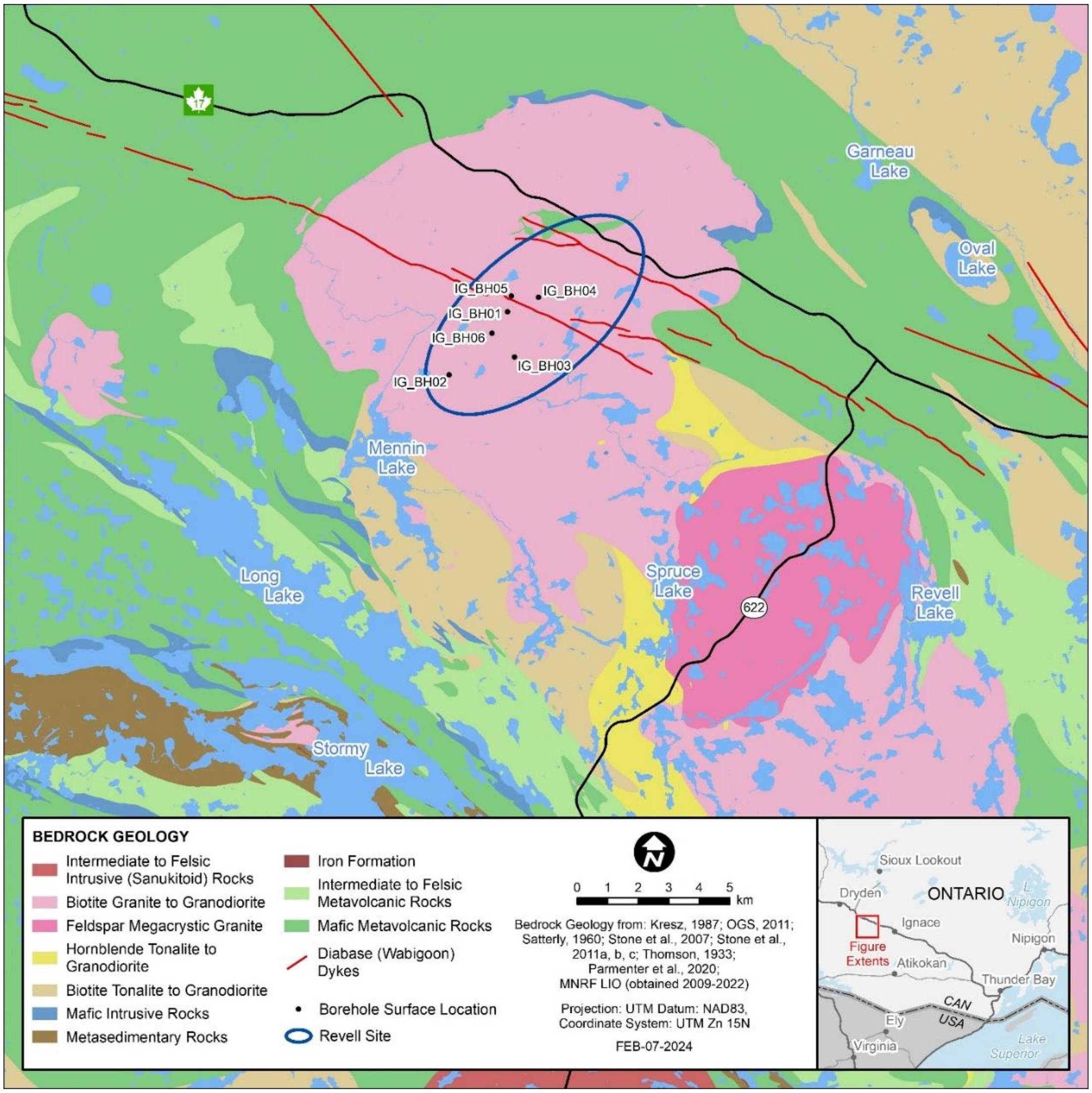

Figure 4-1: Surface Bedrock Map of the Revell area (NWMO 2023)

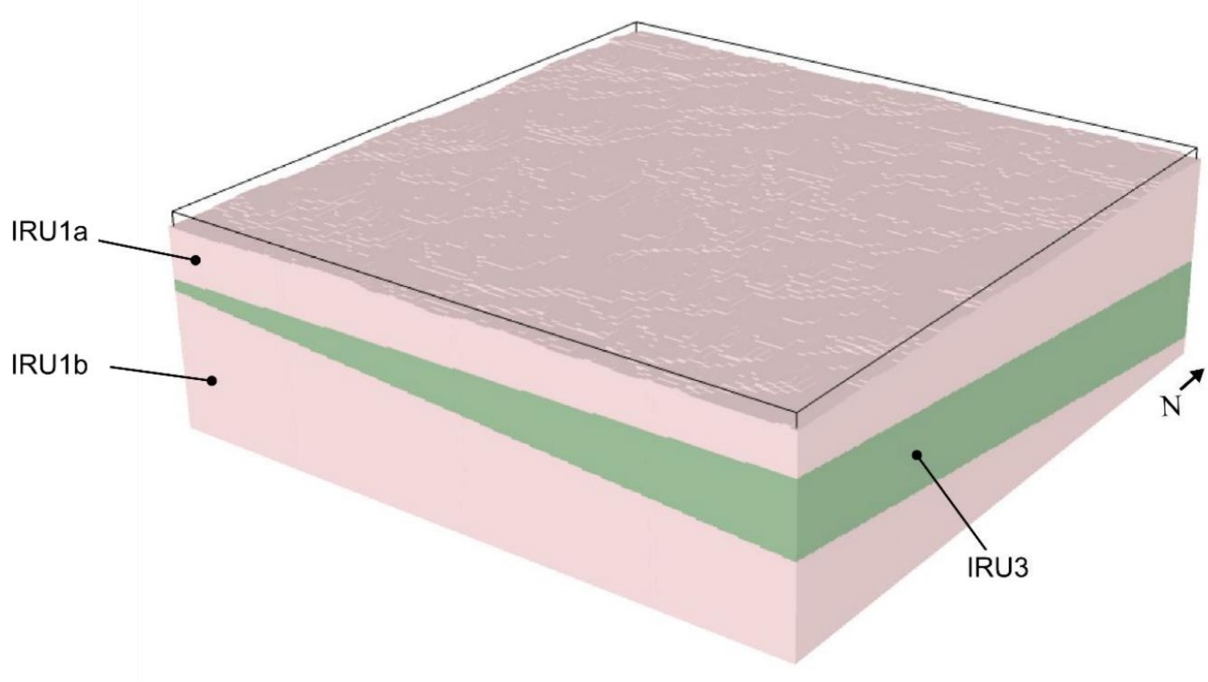

Figure 4-2: Illustration of the ISM-GEO Integrated Rock Units (DesRoches et al. 2021)

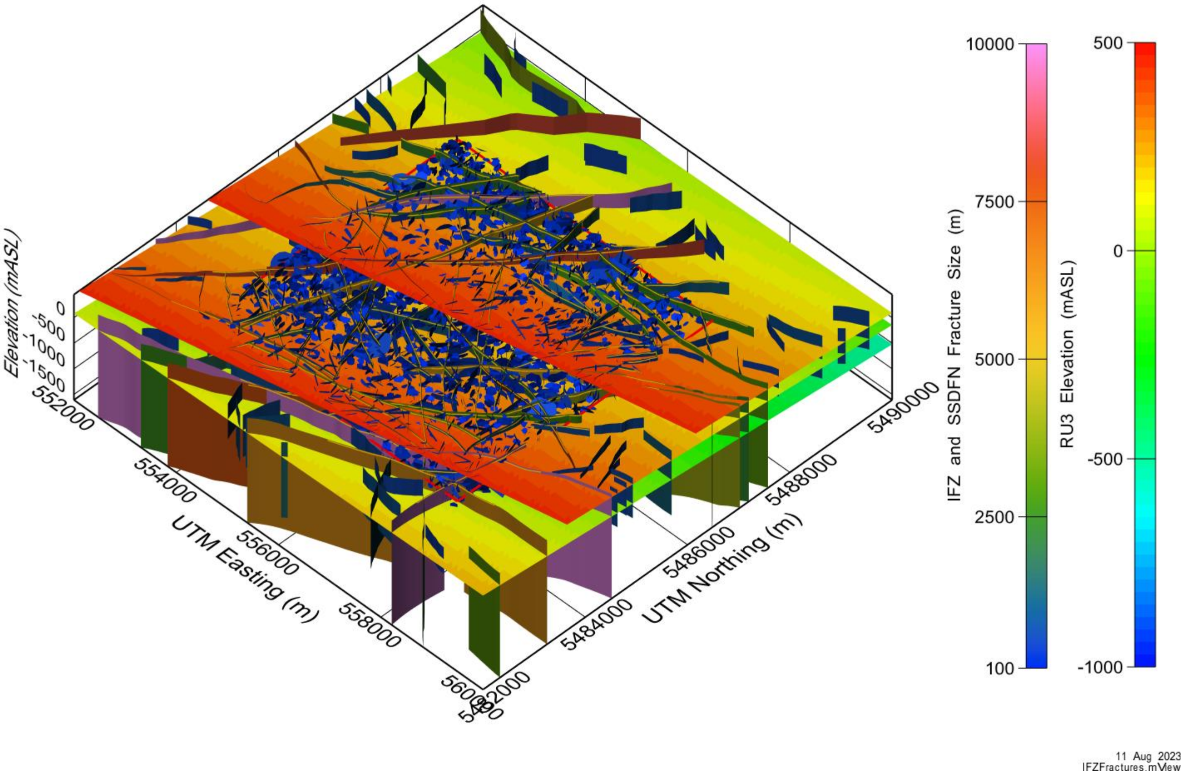

Figure 4-3: Illustration of ISM-GEO Fractures

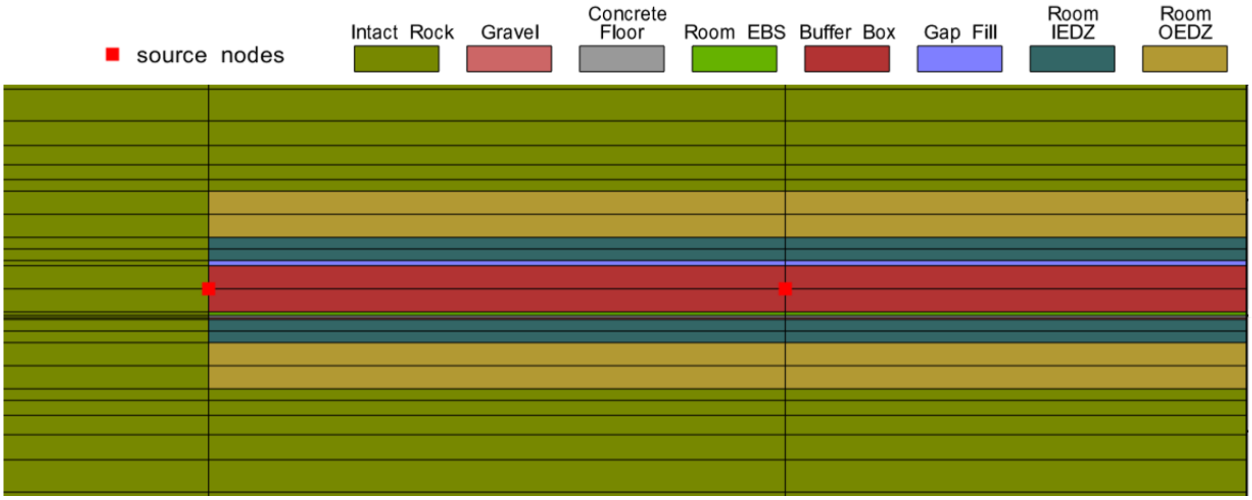

Figure 4-4: Illustration of an ISM-GEO Placement Room

4.3.2 Boundary Conditions

Hydraulic boundary conditions are implemented as fixed heads on the vertical sides and the top of the model. The surface-boundary fixed head is set equal to ground surface elevation. Model side boundary conditions are interpolated from hydraulic head fields calculated from the larger regional scale flow model (Figure 4-5). The model extends to a depth of 1500 m below the ground surface such that the groundwater flow domain affecting the repository is adequately captured. A zero-flow boundary condition is applied to the bottom of the model to ensure that any downward transport of contaminants will be contained within the model domain. Cauchy or third-type transport boundary conditions are applied at all external model boundaries.

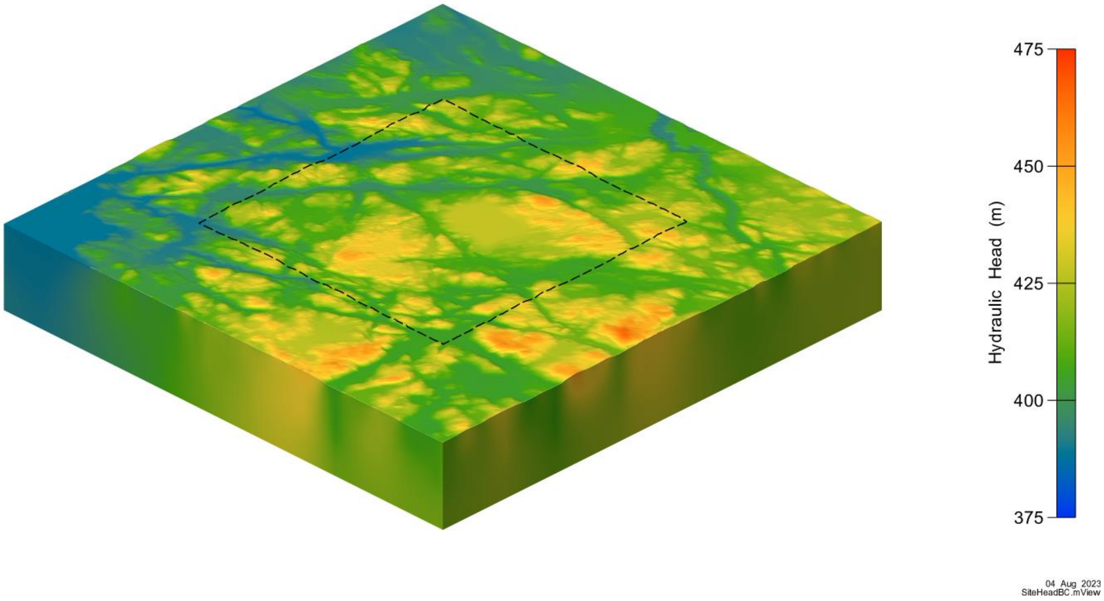

Figure 4-5: ISM-GEO Hydraulic Head Boundary Conditions

4.3.3 Interface with the Wasteform Model

Model source terms are calculated by ISM-WF (see Section 3.2.4) and are defined in terms of mass transport rates for a single-container failure. Specified mass transfer rates are then applied at appropriate source nodes within the ISM-GEO model (see Figure 4-4).

With appropriate source nodes and source term multipliers any combination of used fuel or wasteforms containers can be represented in the ISM-GEO model.

4.3.4 Interface with the ISM-BIO Model

The ISM-GEO model interfaces with the ISM-BIO model by passing transport (integrated flux over an area) for discharge zones of most interest. Discharge zones are defined as follows:

- Watershed areas for surface water features and wetlands are defined based on local topography and determined using the Ontario Flow Assessment Tool (MNRF 2020).
- The region over which discharge to the surface can occur within the regional watershed is determined via transport simulations of the ISM-GEO model and considers potential releases from across the repository.
- For watershed areas containing wetlands all discharge enters the organic wetland sediments.
- If the watershed area is associated with a surface water feature, aquatic and terrestrial components are defined. Aquatic discharge zones are defined as the area within 100 m of a watercourse or waterbody and any defined wetland areas. The terrestrial component of the discharge zone is defined as the area that is not aquatic discharge.

The local surface discharges are nine unnamed lakes referred to as Lake A, Lake B, Lake C, Lake D, Lake E, Lake F, Lake G, Lake H, and Lake I as well as the larger Mennin Lake tributary. Each lake discharge zone has an aquatic (within 100 m of a watercourse or waterbody) and a terrestrial (i.e., not surface water) component associated with the discharge are inputs into the ISM-BIO model. Direct discharge to three wetlands referred to as wetland A, wetland B, and wetland C are also considered.

The ISM-GEO model includes three wells designed to support different biosphere receptors (also referred to as lifestyles). The first well is the well supporting the maximally exposed lifestyle and is conservatively located such that it intercepts the maximum release from the repository. Other wells (municipal or single family) support the site-specific lifestyles and are intended to represent a well a local resident in the Revell area may currently be using as a source of domestic water.

The discharge out of the model boundaries can be used in select downstream compartments in the biosphere model (See Section 5.3 for more details).

The ISM-GEO transport and corresponding ISM-BIO compartments are shown in Table 4-1. Note that the Wabigoon Lake and Michel Lake compartment in the ISM-BIO model are downstream compartments and do not receive discharge directly from the ISM-GEO model.

Table 4-1: ISM-BIO Interfaces with ISM-GEO

ISM-GEO Discharge	ISM-BIO Compartment	Notes
Maximally Exposed Well	Well	Active well(s) in the biosphere depend on the scenario and receptor lifestyle being considered. The maximally exposed well is sited such that it maximizes uptake of contaminants by the well. The single family and community wells are representative of wells typical to the siting region.
Single Family Well		
Community Well(s)		
Lake (A, B, C, D, E, F, G, H, I) – Surface Water	Lake A, B, C, D, E, F, G, H, I	Direct discharge to ISM-BIO from ISM-GEO. The Lake (A, B, C, D, E, F, G, H, I) aquatic discharges in the geosphere model correspond with the Lake (A, B, C, D, E, F, G, H, I) compartments in the biosphere model. The terrestrial discharge is either assumed to enter the garden or forage fields or is conservatively assumed to enter the corresponding Lake compartment (see Section 5.2.2.1.1).
Lake (A, B, C, D, E, F, G, H, I) – Terrestrial		
Wetland (A, B, C)	Wetland A, B, C	Direct discharge to ISM-BIO from ISM-GEO. The Wetland (A, B, C) discharge in the geosphere model correspond with the Wetland (A, B, C) compartment in the biosphere model. (see Section 5.2.10.1.1).
Mennin Lake Tributary Surface Water	Mennin Lake	Direct discharge to ISM-BIO from ISM-GEO. The Mennin Lake Tributary aquatic discharge in the geosphere model correspond with the Mennin Lake Tributary compartment in the biosphere model. The terrestrial discharge is either assumed to enter the garden or forage fields or is conservatively assumed to enter the Mennin Lake Tributary (see Section 5.2.2.1.1).
Mennin Lake Tributary Terrestrial		
Dinorwic Lake – Surface Water	Dinorwic Lake	This is a downstream compartment in the ISM-BIO model and receives all discharge from the ISM-GEO model that does not enter the Wells, Lakes and Mennin Lake Tributary discharges described above.
None	Wabigoon Lake	The Wabigoon Lake compartment in the ISM-BIO model is downstream of the Dinorwic Lake compartment and does not receive any input from the ISM-GEO model.

ISM-GEO Discharge	ISM-BIO Compartment	Notes
None	Michel Lake	The Michel Lake compartment represent an Isolated surface water feature in the ISM-BIO model that does not receive input from ISM-GEO model but may be used as a source of water for select lifestyles.
User Defined	Forage Field	Proportional to terrestrial component of main surface water discharge (see Section 5.2.2.1.1 and 5.2.8.1.1).
User Defined	Garden Field	Proportional to terrestrial component of main surface water discharge (see Section 5.2.2.1.1 and 5.2.8.1.1).

The discharge to the forage and garden fields are treated as a special case in the ISM-BIO model. Each surface water discharge (e.g., Lake A) has an associated terrestrial discharge in the ISM-GEO. The garden and forage fields receive discharge from the terrestrial discharge associated with the main surface waterbody (See Section 5.2.2) and proportional to the area of fields (See Section 5.2.8). A field does not receive discharge from the geosphere if the field is irrigated as it would maintain a positive water balance and inhibit upward movement of groundwater.

5. BIOSPHERE MODEL

5.1 Biosphere Model Overview

The biosphere (also referred to as the ISM-BIO model) describes the movement of contaminants (radionuclides and stable elements) in the surface environment after release from the geosphere, and the consequent radiological dose and non-radiological consequences to a variety of lifestyles including a maximally exposed lifestyle. ISM-BIO model represents the Revell site and is implemented in AMBER, which is a compartment modelling software developed by Quintessa Ltd (Quintessa 2023). The models assume that compartments are instantaneously homogenously mixed as contaminants are transferred from one compartment to the next.

The equations that define the biosphere models in the ISM-BIO model are predominantly based on the CSA N288.1:20 model (CSA 2020). It is noted that the CSA N288.1:20 standard is intended to provide guidelines for calculating derived release limits for airborne and liquid effluents for normal operations of nuclear facilities, and therefore the release points of contaminants are different compared with a deep geological repository (i.e., airborne stack release and liquid effluent from a facility versus geosphere discharge). The ISM-BIO model includes many of the CSA N288.1:20 processes, with some notable exceptions, such as releases from an airborne stack and releases of liquid effluents to surface water.

Another key difference between the ISM-BIO model and the CSA N288.1:20 model is that CSA N288.1:20 is not a dynamic model. That is, it assumes steady release and an equilibrium between biosphere components. The ISM-BIO model calculates concentration of contaminants in soil and surface waters, by allowing for dynamic transfer of contaminants between media, and to accommodate a time-varying release rate from the geosphere into the biosphere. Concentrations in other biosphere components are calculated assuming steady release and equilibrium between components as in CSA N288.1:20.

All dose pathways considered in CSA N288.1:20 are included in the ISM-BIO model.

5.2 General Biosphere Model Theory

This section describes the general biosphere model theory.

5.2.1 Well Water Concentration

This section describes the concentration of contaminants in well water for wells included in the biosphere models. Lifestyles can include a residential well, a community well, or both residential and community wells in some lifestyles. An example of a scenario of when both wells are considered is the local resident lifestyle. In this lifestyle the domestic water source (drinking, cooking, bathing) can be a community well, however the receptor may also ingest produce or livestock products from a local farm which uses a residential well for watering livestock and irrigation.

5.2.1.1 Residential Well Water Concentration

The well water concentration for a residential well is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(\mathrm{t}) = \frac{\mathrm{X}^{\mathrm{j}}_{\mathrm{well,r}}(\mathrm{t})}{Q^{l}_{well} \cdot \rho_{\mathrm{wat}}} \tag{5-1}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(t)$	is the concentration of contaminant j in the residential well [mol/kg$_{\text{water}}$];
$\mathrm{X}^{\mathrm{j}}_{\mathrm{well,r}}(t)$	is the discharge rate from geosphere to the residential well for contaminant j [mol/a];
Q^{l}_{well}	is the total well demand [m$^{3}_{\text{water}}$/a] for a lifestyle using a residential well; and
ρ_{wat}	is the water density [kg$_{\text{water}}$/m$^{3}_{\text{water}}$].

The total well demand depends on the domestic water demand, the livestock water demand, the irrigation water demand and the well capacity. If the well capacity can meet the domestic water, livestock and irrigation needs (i.e., $Q^{l}_{cap} \geq Q^{l}_{dom} + Q^{l}_{ls} + Q^{l}_{irr}$), then the total well demand is:

$$\mathbf{Q}^{\boldsymbol{l}}_{\boldsymbol{well}} = \mathbf{Q}^{\boldsymbol{l}}_{\boldsymbol{dom}} + \mathbf{Q}^{\boldsymbol{l}}_{\boldsymbol{ls}} + \mathbf{Q}^{\boldsymbol{l}}_{\boldsymbol{irr}} \tag{5-2}$$

where,

Q^{l}_{well}	is the total well demand [m$^{3}_{\text{water}}$ /a] for lifestyle l;
Q^{l}_{dom}	is the domestic water demand [m$^{3}_{\text{water}}$ /a] for lifestyle l given by Equation (5-3);
Q^{l}_{ls}	is the livestock water demand [m$^{3}_{\text{water}}$ /a] for lifestyle l given by Equation (5-4);
Q^{l}_{irr}	is the irrigation water demand [m$^{3}_{\text{water}}$ /a] for lifestyle l given by Equation (5-5);
Q^{l}_{cap}	is the capacity of the well to provide water [m$^{3}_{\text{water}}$ /a] in lifestyle l;

The domestic water demand Q^{l}_{dom} is defined as:

$$\mathrm{Q}^{l}_{dom} = \mathrm{N}^{l}_{ppl} \cdot \mathrm{Q}^{l}_{dw} \cdot \delta^{l}_{well,dom} \tag{5-3}$$

where,

Q^{l}_{dom}	is the domestic water demand [m$^{3}_{\text{water}}$/a] for lifestyle l;
N^{l}_{ppl}	is the number of people in the lifestyle group [-];
Q_{dw}	is the annual domestic water demand per person [m$^{3}_{\text{water}}$/ (person·a)] for lifestyle l; and
$\delta^{l}_{well,dom}$	is a Boolean parameter that is 1 if the well is used for domestic use water in lifestyle l and 0 if a different source of domestic use water is used in lifestyle l.

The livestock water demand Q^{l}_{ls} is defined as:

$$\mathrm{Q}^{l}_{ls} = \sum_{\mathrm{ls}} \left(\frac{\mathrm{N}^{l}_{ls} \cdot \mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,wat}}}{\rho_{wat}} \right) \cdot \delta^{l}_{well,ls} \tag{5-4}$$

where,

Q^{l}_{ls}	is the domestic water demand [m$^{3}_{\text{water}}$/a] for livestock ls;
N^{l}_{ls}	is the number of livestock ls [-] defined in Equation (5-28) for lifestyle l;
$\mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,wat}}$	is the livestock ingestion rate of water [kg$_{\text{water}}$/a] for livestock ls;
ρ_{wat}	is the density of water [kg$_{\text{water}}$/m$^{3}_{\text{water}}$]; and

$\delta_{well,ls}^{l}$	is a Boolean parameter that is 1 if the well is used for watering livestock in lifestyle l and 0 if a different source of water is used for watering livestock or livestock are not a component of lifestyle l.

The irrigation water demand ($\mathrm{Q_{irr}}$) is defined as:

$$Q_{irr}^{l} = \sum_{f} \mathrm{R_{irr,f}^{\mathit{l}}} \cdot \mathrm{A}_{f}^{l} \cdot \delta_{well,irr,f}^{l} \tag{5-5}$$

where,

Q_{irr}	is the irrigation water demand [$\mathrm{m^3_{water}/a}$];
$\mathrm{R_{irr,f}^{\mathit{l}}}$	is the irrigation rate of field f [$\mathrm{m^3_{water}/(m^2_{soil}\ a)}$]; and
A_{f}^{l}	is the area of field f for lifestyle l[$\mathrm{m^2_{soil}}$]; and
$\delta_{well,irr,f}^{l}$	is a Boolean parameter that is 1 if the well is used to irrigate field f in lifestyle l and 0 if a different source of water is used to irrigate field f or if fields are not irrigated in lifestyle l.

If the well cannot meet the water demand of a lifestyle (i.e., $Q_{cap}^{l} < Q_{well}^{l}$) then the well annual flow is limited to its capacity:

$$\mathrm{Q}_{well}^{l} = \mathrm{Q}_{cap}^{l} \tag{5-6}$$

If the well cannot adequately support the water demand of a given lifestyle, other sources of water such as surface waters may be used to supplement the well (see Section 5.2.2).

5.2.1.2 Community Well Concentration

Some lifestyles may draw their domestic use water (for drinking, cooking, bathing) from a community well. The well water concentration for a community well is given by:

$$\mathrm{C_{well,c}^{j,l}(t)} = \frac{\mathrm{X_{well,c}^{j}(t)}}{Q_{cwd}^{l} \cdot \mathrm{\rho_{wat}}} \tag{5-7}$$

where,

$\mathrm{C_{well,c}^{j,l}}(t)$	is the concentration of contaminant j in the community well [$\mathrm{mol/kg_{water}}$];
$\mathrm{X_{well,c}^{j}}(t)$	is the discharge rate from geosphere to the community well for contaminant j [mol/a];
Q_{cwd}^{l}	is the total community well demand [$\mathrm{m^3_{water}/a}$]; and
$\mathrm{\rho_{wat}}$	is the water density [$\mathrm{kg_{water}/m^3_{water}}$].

The community well is expected to have a capacity much greater than the domestic needs of the lifestyle group being considered (i.e. $Q_{cap}^{l} \gg Q_{dom}^{l}$). Consequently, supplementary water sources are not considered when domestic water is drawn from a community well.

5.2.2 Surface Water Concentration

Contaminants are discharged from the geosphere to one or more surface water features or topographical low points. The ISM-BIO model includes several surface waterbodies. Surface waterbodies include lakes, rivers, and wetlands. The geosphere model determines the amounts of contaminated water discharged to each of these waterbodies (see Section 4.3.4). The transport processes included in the model are illustrated in Figure 5-1.

The domestic surface waterbody is the surface water feature from which the lifestyles will draw on for their household domestic water needs (e.g., drinking, cooking, bathing) if a well is not used. The domestic surface waterbody may also be used to supplement the domestic water needs of a lifestyle with a residential well if the well capacity is less than the domestic water demand. The main surface waterbody is the surface waterbody used in a lifestyle for fishing, hunting and gathering. The main surface waterbody may also be used as the source of water for watering livestock and irrigating fields if a residential well is not used. Finally, the main surface waterbody can also be used to supplement a residential well used for irrigation and watering of livestock if the well capacity is less than the livestock watering and irrigation water demands for a lifestyle.

The domestic surface waterbody and main surface waterbody are specified in the biosphere model input file. The main surface waterbody can also be dynamically calculated such that the most contaminated surface waterbody is automatically selected.

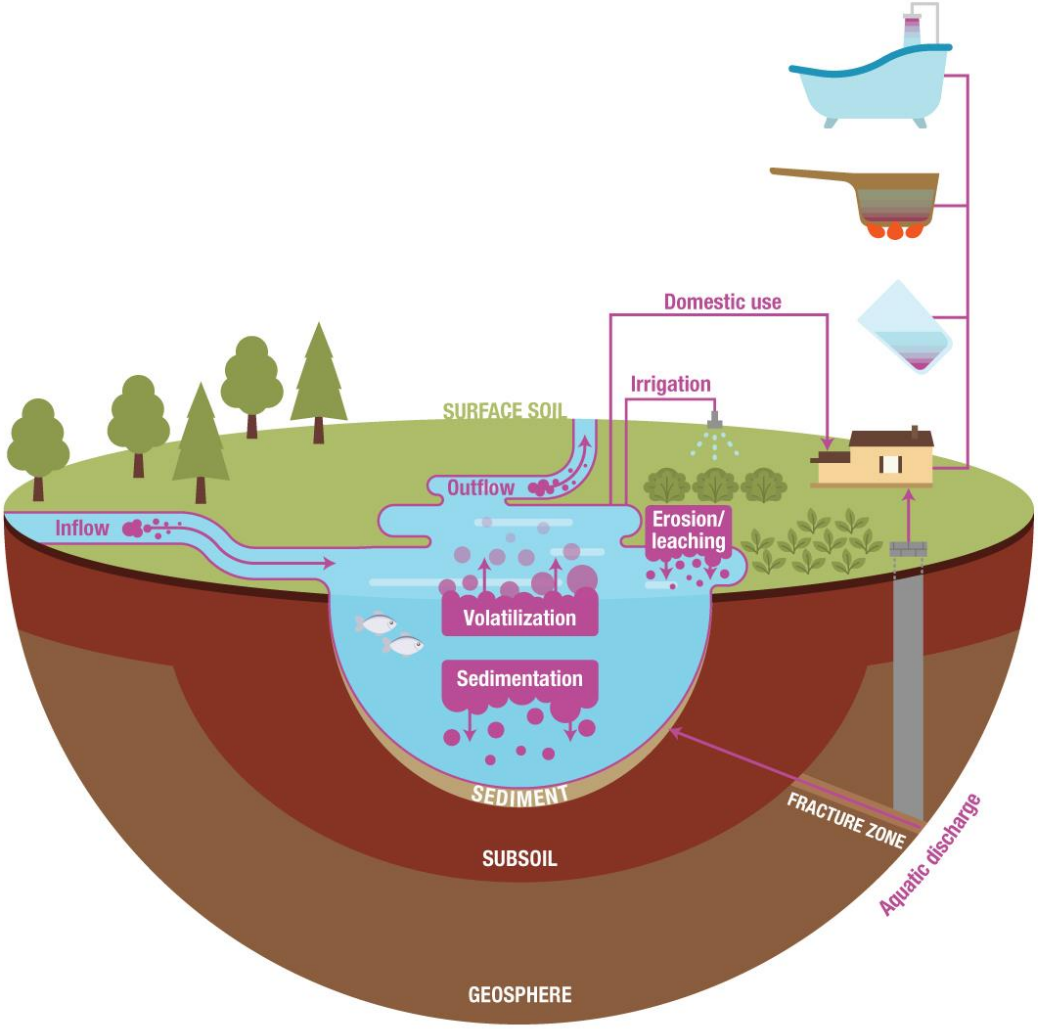

Figure 5-1: Surface Water Transport Processes

5.2.2.1 Surface Water Sources

The biosphere models consider four pathways for contaminants to enter the surface water features. The first pathway is by direct discharge from the geosphere. These release rates are calculated by the geosphere model for discharge zones (see Section 4.3.4). The second pathway is the inflow of contaminated water from other surface water features. The third pathway is from discharge of the domestic and livestock water used by a given lifestyle and the fourth is from nearby soils via processes like erosion and leaching.

5.2.2.1.1 Discharge to Lakes and Rivers

The transport to each surface water feature is determined by the geosphere model (see Section 4.3.4). Discharge from the geosphere associated with each waterbody has two components an aquatic portion and a terrestrial portion.

For the main surface waterbody, the aquatic portion of the discharge from the geosphere and a fraction of the terrestrial discharge from the geosphere is assumed to enter the waterbody in the biosphere. For the terrestrial discharge from the geosphere a fraction of the discharge enters the garden and forage fields associated with the main surface waterbody (see Section 5.2.8.1.1) and would eventually mix with the surface waterbody via leaching (see Section 5.2.8.2.1). The remainder of the terrestrial discharge associated with the main surface waterbody would enter soils outside the garden and forage fields and would also eventually mix with the main surface waterbody via leaching as well. Conservatively the remainder of the terrestrial discharge from the main surface waterbody is assumed to enter the main surface waterbody directly.

Other waterbodies do not have fields associated with them and therefore all discharge from the geosphere (aquatic and terrestrial) are assumed to enter the surface waterbody directly. Specifically:

$$\mathrm{X}^{j}_{sw,\mathrm{tot}}(\mathrm{t}) = \mathrm{X}^{j}_{\mathrm{sw,D}}(\mathrm{t}) + \delta^{l}_{msw}\left(1 - \mathrm{f}^{l}_{soil}\right)\mathrm{X}^{j}_{\mathrm{ter,D}}(\mathrm{t}) + \left(1 - \delta^{l}_{msw}\right)\mathrm{X}^{j}_{\mathrm{ter,D}}(\mathrm{t}) \tag{5-8}$$

where,

$\mathrm{X}^{j}_{\mathrm{sw,tot}}(\mathrm{t})$	is the total transport from the geosphere for contaminant j to surface water feature sw [mol/a];
$\mathrm{X}^{j}_{\mathrm{sw,D}}(\mathrm{t})$	is the surface water component of the transport from the geosphere model to discharge D [mol/a];
$\mathrm{X}^{j}_{\mathrm{ter,D}}(\mathrm{t})$	is the terrestrial component of the transport from the geosphere model to discharge D [mol/a];
δ^{l}_{msw}	is a Boolean parameter that is 1 if the surface water feature is the main surface waterbody for lifestyle l and 0 if the discharge is not the main surface waterbody; and
$\mathrm{f}^{\mathrm{l}}_{\mathrm{soil}}$	is the fraction of the terrestrial component of the transport from the geosphere entering the garden and forage field soils for lifestyle l defined in Equation (5-24).

5.2.2.1.2 Flow between Surface Water Features

The rate at which contaminants are transferred from one upstream surface water feature (e.g., lakes, rivers, wetlands) to a downstream feature is modelled as follows:

$$\lambda^{j}_{inflow,sw}(\mathrm{t}) = \frac{N^{j}_{sw-1}(\mathrm{t}) \cdot \mathrm{Q}_{\mathrm{flow,sw-1}}}{\mathrm{V}_{sw-1}} \tag{5-9}$$

where,

$\lambda^{j}_{inflow,sw}(\mathrm{t})$	is the transfer rate of contaminant j from the upstream surface water feature to the surface water feature sw [mol/a];
$N^{j}_{sw-1}(\mathrm{t})$	is the amount of contaminant j in the upstream surface waterbody (sw-1) as determined by the biosphere model [mol];
$\mathrm{Q}_{\mathrm{flow,sw-1}}$	is a model input. It represents the total volumetric water flow rate from the upstream water feature (sw-1) to the downstream water feature [$\mathrm{m}^3_{\mathrm{water}}$/a] or to the sink and should consider all water flow sources to the upstream water body (runoff, upstream waterbodies and groundwater discharge); and
$\mathrm{V}_{\mathrm{sw-1}}$	is the volume of the upstream waterbody [$\mathrm{m}^3_{\mathrm{water}}$].

5.2.2.1.3 Discharge of Domestic and Livestock Water

For lifestyles that include a residential well, all water used for domestic purposes and for watering livestock are conservatively assumed to discharge into the main surface waterbody. The rate at which contaminants are transferred from domestic water to the main surface waterbody is modelled as follows.

$$\mathrm{X}^{\mathrm{j,l}}_{\mathrm{msw,dom}}(\mathrm{t}) = \mathrm{X}^{\mathrm{j}}_{\mathrm{well,r}}(\mathrm{t}) \cdot \frac{\mathrm{f}^{\mathrm{l}}_{\mathrm{dom+ls,well}} \cdot \left(Q^{l}_{dom} + Q^{l}_{ls}\right)}{\mathrm{Q}^{l}_{well}} \tag{5-10}$$

where,

$\mathrm{X}^{\mathrm{j,l}}_{msw,dom}(t)$	is the transport of contaminant j from the well to the main surface waterbody for lifestyle l [mol/a];
$\mathrm{X}^{\mathrm{j}}_{\mathrm{well,r}}(t)$	is the discharge rate of contaminant j from geosphere to the residential well [mol/a];
$\mathrm{f}^{\mathrm{l}}_{\mathrm{dom+ls,well}}$	is the fraction domestic and livestock water that is taken from the well for lifestyle l defined in Equation (5-11);
Q^{l}_{well}	is the total well demand [$\mathrm{m}^3_{\mathrm{water}}$/a] for lifestyle l described in Section 5.2.1;
Q^{l}_{dom}	is the domestic water demand [$\mathrm{m}^3_{\mathrm{water}}$/a] for lifestyle l given by Equation (5-3); and
Q^{l}_{ls}	is the livestock water demand [$\mathrm{m}^3_{\mathrm{water}}$/a] for lifestyle l given by Equation (5-4).

The fraction of domestic and livestock water that is taken from the well is given by:

$$\mathrm{f}^{\mathrm{l}}_{\mathrm{dom+ls,well}} = \begin{cases} 1 & \text{if } \mathrm{Q}_{\mathrm{cap}} \geq Q^{l}_{dom} \text{ and } \delta^{l}_{well,dom} \text{ or } \delta^{\mathrm{l}}_{\mathrm{well,ls}} = 1 \\ \mathrm{Q}_{\mathrm{cap}} / \left(Q^{l}_{dom} + Q^{l}_{ls}\right) & \text{if } \mathrm{Q}_{\mathrm{cap}} < Q^{l}_{dom} \text{ and } \delta^{l}_{well,dom} \text{ or } \delta^{\mathrm{l}}_{\mathrm{well,ls}} = 1 \\ 0 & \text{if } \mathrm{Q}_{\mathrm{cap}} = 0 \text{ or } \delta^{l}_{well,dom} \text{ and } \delta^{\mathrm{l}}_{\mathrm{well,ls}} = 0 \end{cases} \tag{5-11}$$

where,

$\mathrm{Q}_{\mathrm{cap}}$	is the annual well capacity [$\mathrm{m}^3_{\mathrm{water}}$/a];

Q_{dom}^{l}	is the domestic water demand [m^3_{water} /a] for lifestyle l given by Equation (5-3);
$\delta_{well,dom}^{l}$	is a Boolean parameter that is 1 if the well is used for domestic use water in lifestyle l and 0 if a different source of domestic use water is used in lifestyle l; and
$\delta_{well,dom}^{l}$	is a Boolean parameter that is 1 if the well is used for livestock water in lifestyle l and 0 if a different source of livestock water is used.

5.2.2.1.4 Flow from Surface Soil

Transport to the main surface waterbody from the forage field and garden field via leaching and erosion are described in Section 5.2.8.2.1 and Section 5.2.8.2.2 respectively.

5.2.2.2 Losses from Surface Water Features

Losses from surface water features included in the biosphere model are loss to other downstream surface water features, volatilization, and sedimentation. These loss terms are broadly applicable to multiple surface water features (i.e., lakes, rivers, and wetlands) and surface water features will be differentiated through parameter values. For example, a wetland or lake may have a higher sedimentation rate than a river.

5.2.2.2.1 Flow between Surface Water Features and Wetlands

The transfer of contaminants between surface waterbodies and wetlands is described in Section 5.2.2.1.2 and by Equation (5-9).

5.2.2.2.2 Volatilization

Contaminants can enter the atmosphere from surface water via volatilization. This process is described as a loss from the system (i.e., transfer to the sink). Loss from the surface water is modelled assuming a water volatilization rate constant and the loss rate from a given surface water feature is given by:

$$\lambda_{vol,sw}^{j}(\mathrm{t}) = N_{sw}^{j}(\mathrm{t}) \cdot \mathrm{VR}_{wat}^{j} \tag{5-12}$$

where,

$\lambda_{vol,sw}^{j}(\mathrm{t})$	is the loss rate of contaminant j from surface water feature sw due to volatilization [mol/a];
$N_{sw}^{j}(\mathrm{t})$	is the amount of contaminant j in the surface water feature (compartment) sw at time t as calculated by the biosphere model [mol]; and
VR_{wat}^{j}	is the water volatilization rate constant for contaminant j [a^{-1}].

5.2.2.2.3 Sedimentation

Contaminants can be removed from the water column via sedimentation. In the ISM, this process is described as a loss from the system (i.e., transfer to the sink), not as a transfer to a sediment compartment. Loss from the surface water due to sedimentation is dependent on the sediment solid-to-liquid partition coefficient ($\mathrm{kd}_{\mathrm{sed}}^{\mathrm{j}}$) and the equation for the sedimentation rate is described in Clause 6.6.2.2 of CSA (2020) and is given by:

$$\lambda^{\mathrm{j}}_{\mathrm{sed,sw}}(\mathrm{t}) = \frac{N^{j}_{sw}(\mathrm{t}) \cdot \mathrm{DR}_{sw} \cdot \rho_{\mathrm{sed}} \cdot \mathrm{A}_{sed} \cdot \mathrm{kd}^{\mathrm{j}}_{\mathrm{sed}}}{\mathrm{V}_{\mathrm{sw}}} \tag{5-13}$$

where,

$\lambda^{\mathrm{j}}_{\mathrm{sed,sw}}$ (t)	is the loss rate of contaminant j from surface water feature sw due to sedimentation [mol/a];
$N^{j}_{sw}(\mathrm{t})$	is the amount of contaminant j in the surface water (compartment) sw as determined by the biosphere model [mol];
DR_{sw}	is the sediment accumulation rate for a given surface water feature [$\mathrm{m}^3_{\mathrm{sediment}}$/($\mathrm{m}^2_{\mathrm{sediment}}$ a)];
ρ_{sed}	is the density of sediment [$\mathrm{kg}_{\mathrm{sediment\text{-}dw}}$/$\mathrm{m}^3_{\mathrm{sediment}}$];
$\mathrm{A}_{\mathrm{sed}}$	is the surface area of the sediment [$\mathrm{m}^2_{\mathrm{sediment}}$];
$\mathrm{kd}^{\mathrm{j}}_{\mathrm{sed}}$	is the solid-to-liquid partition coefficient for sediment for contaminant j [$\mathrm{m}^3_{\mathrm{water}}$/$\mathrm{kg}_{\mathrm{sediment\text{-}dw}}$]; and
V_{sw}	is the volume of the surface water feature sw [$\mathrm{m}^3_{\mathrm{water}}$].

A more detailed modelling of transfer between the sediments and surface waters will be developed as the site characterization process continues.

5.2.2.3 Surface Water Concentration

The concentration of contaminant is calculated from the amount of contaminant in the surface water body compartment. The amount of contaminant is calculated by AMBER numerically as the sum of sources, inflows and subtraction of outflows and decay. The equation applied in amber is:

$$\begin{aligned}
\mathrm{N}^{\mathrm{j}}_{\mathrm{sw}}(t) = \mathrm{N}^{\mathrm{j}}_{\mathrm{sw}}(t^{-1}) \\
&+ \Delta\mathrm{t}\Bigg[\mathrm{X}^{j}_{sw,\mathrm{tot}}(t^{-1}) + \Bigg(\sum_{up\ sw} \lambda^{j}_{inflow,sw}(t^{-1})\Bigg) \\
&+ \delta^{l}_{msw}\left(\lambda^{j}_{vol,sw}(t^{-1}) + \lambda^{j}_{er,f}(t^{-1}) + \mathrm{X}^{\mathrm{j,l}}_{msw,dom}(t^{-1})\right) \\
&- \Bigg(\sum_{down\ sw} \lambda^{j}_{outflow,sw}(t^{-1})\Bigg) - \lambda^{\mathrm{j}}_{\mathrm{sed,sw}}(t^{-1}) - \lambda^{j}_{vol,sw}(t^{-1}) \\
&- \lambda^{j}_{dec}\mathrm{N}^{\mathrm{j}}_{w}(t^{-1})\Bigg]
\end{aligned} \tag{5-14}$$

where,

$\mathrm{N}^{\mathrm{j}}_{\mathrm{sw}}$	is the amount of contaminant j in the surface water (compartment) sw as determined by the biosphere model [mol];
$\lambda^{\mathrm{j}}_{\mathrm{leach,f}}$	is the leaching rate of contaminant j from field f [mol/a];
$\lambda^{j}_{er,f}$	is the erosive rate of contaminant j from field f [1/a];
$\mathrm{X}^{j}_{\mathrm{sw,tot}}$	is the total transport from the geosphere for contaminant j to surface water feature sw [mol/a];
δ^{l}_{msw}	is a Boolean parameter that is 1 if the surface water feature is the main surface waterbody for lifestyle l and 0 if the discharge is not the main surface waterbody;

$X^{j,l}_{msw,dom}$	is the transport of contaminant j from the well to the main surface waterbody for lifestyle l [mol/a];
$\lambda^{j}_{sed,sw}$	is the loss rate of contaminant j from surface water feature sw due to sedimentation [mol/a];
$\lambda^{j}_{vol,sw}$	is the loss rate of contaminant j from surface water feature sw due to volatilization [mol/a];
$\lambda^{j}_{inflow,sw}$	is the transfer rate of contaminant j from the upstream surface water feature to the surface water feature sw [mol/a];
$\lambda^{j}_{outflow,sw}$	is the transfer rate of contaminant j from the surface water feature sw to a downstream surface water feature [mol/a]; and
λ^{j}_{dec}	is the decay constant of contaminant j [1/a].

The concentration of contaminant j in a surface water feature is then calculated as follows:

$$C^{j}_{sw}(t) = \frac{N^{j}_{sw}(t)}{V_{sw} \cdot \rho_{wat}} \tag{5-15}$$

where,

$C^{j}_{sw}(t)$	is concentration of contaminant j in surface water feature sw [mol/kg$_{water}$];
N^{j}_{sw}	is the amount of contaminant j in the surface water (compartment) sw as determined by the biosphere model [mol];
V_{sw}	is the volume of the surface water feature sw [m$^3_{water}$]; and
ρ_{wat}	is the density of water [kg/m$^3_{water}$].

As noted in Section 5.2.2, the user can specify a domestic surface waterbody and a main surface waterbody for a lifestyle. The concentration in the main surface waterbody is determined by:

$$C^{j,l}_{msw}(t) = \sum_{sw} \delta^{l}_{msw} \cdot C^{j}_{sw}(t) \tag{5-16}$$

where,

$C^{j,l}_{msw}$	is concentration of contaminant j in the main surface waterbody for lifestyle l [mol/kg$_{water}$];
δ^{l}_{msw}	is a Boolean parameter that is 1 if a surface water feature is selected by the user to be the main surface waterbody for lifestyle l or 0 if the surface water feature is not the main surface waterbody; and
C^{j}_{sw}	is concentration of contaminant j in surface water feature sw [mol/kg$_{water}$] given by Equation (5-15).

Similarly, the concentration in the domestic surface waterbody is determined by:

$$C^{j,l}_{dsw}(t) = \sum_{sw} \delta^{l}_{dsw} \cdot C^{j}_{sw}(t) \tag{5-17}$$

where,

$\mathrm{C}_{\mathrm{dsw}}^{\mathrm{j,l}}$	is concentration of contaminant j in the domestic surface waterbody for lifestyle l [mol/kg$_{\mathrm{water}}$];
δ_{dsw}^{l}	is a Boolean parameter that is 1 if a surface waterbody is selected by the user to be the domestic surface waterbody for lifestyle l and 0 if the surface water feature is not the domestic surface waterbody; and
$\mathrm{C}_{\mathrm{sw}}^{\mathrm{j}}$	is concentration of contaminant j in surface water feature sw [mol/kg$_{\mathrm{water}}$] given by Equation (5-15).

5.2.3 Domestic Water Concentration

The domestic water is the water used by a lifestyle for activities such as drinking, cooking and bathing. This water can come from a community well, a residential well, the domestic surface waterbody, or some combination of the residential well and the domestic surface waterbody sources depending on the lifestyle. The domestic water concentration is given by:

$$\begin{aligned}\mathrm{C}_{\mathrm{dom}}^{\mathrm{j,l}}(t) = {} & \delta_{well,c}^{l}\mathrm{C}_{\mathrm{well,c}}^{\mathrm{j,l}}(t) \\ & + \left(1-\delta_{well,c}^{l}\right)\left(\mathrm{f}_{dom+ls,well}^{l}\mathrm{C}_{\mathrm{well,r}}^{\mathrm{j,l}}(t) + \left(1-\mathrm{f}_{\mathrm{dom+ls,well}}^{l}\right)\mathrm{C}_{\mathrm{dsw}}^{\mathrm{j,l}}(t)\right)\end{aligned} \tag{5-18}$$

where,

$\mathrm{C}_{\mathrm{dom}}^{\mathrm{j,l}}(t)$	is the domestic use water concentration of contaminant j and lifestyle l [mol/kg$_{\mathrm{water}}$];
$\delta_{well,c}^{l}$	is a Boolean parameter that is 1 if a community well is used as the source of domestic water for a lifestyle or 0 if it is not used;
$\mathrm{C}_{\mathrm{well,r}}^{\mathrm{j,l}}(t)$	is the concentration of contaminant j in the residential well for lifestyle l [mol/kg$_{\mathrm{water}}$] given by Equation (5-1).
$\mathrm{C}_{\mathrm{dsw}}^{\mathrm{j,l}}(t)$	is the concentration of contaminant j in the domestic surface water feature [mol/kg$_{\mathrm{water}}$] given by Equation (5-17); and
$\mathrm{f}_{\mathrm{dom+ls,well}}^{l}$	is the fraction of domestic water that is sourced from the residential well [-] for lifestyle l defined in Equation (5-11).

5.2.4 Livestock Water Concentration

The livestock water is the water used by a lifestyle to water the livestock they consume. This water can come from a residential well, the main surface waterbody, or some combination of the two sources depending on the lifestyle and is given by:

$$\mathrm{C}_{lw}^{\mathrm{j,l}}(t) = \mathrm{f}_{dom+ls,\mathrm{well}}^{l}\mathrm{C}_{\mathrm{well,r}}^{\mathrm{j,l}}(t) + \left(1-\mathrm{f}_{dom+ls,\mathrm{well}}^{l}\right)\mathrm{C}_{\mathrm{msw}}^{\mathrm{j,l}}(t) \tag{5-19}$$

where,

$\mathrm{C}_{\mathrm{lw}}^{\mathrm{j,l}}(t)$	is the livestock water concentration of contaminant j and lifestyle l [mol/kg$_{\mathrm{water}}$];
$\mathrm{C}_{\mathrm{well,r}}^{\mathrm{j,l}}(t)$	is the concentration of contaminant j in the residential well for lifestyle l [mol/kg$_{\mathrm{water}}$] given by Equation (5-1).
$\mathrm{C}_{\mathrm{msw}}^{\mathrm{j,l}}(t)$	is the concentration of contaminant j in the main surface waterbody [mol/kg$_{\mathrm{water}}$] given by Equation (5-16);

$\mathrm{f}^{l}_{\mathrm{dom+ls,well}}$	is the fraction of domestic and livestock water that is sourced from the well [-] for lifestyle l defined in Equation (5-11).

5.2.5 Irrigation Water Concentration

In lifestyles where the fields are irrigated, water is sourced from either the residential well, the main surface waterbody, or some combination of the two sources depending on the lifestyle and is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{irr}}(t) = \mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr}} \cdot \mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(t) + \left(1 - \mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr,f}}\right) \cdot \mathrm{C}^{\mathrm{j,l}}_{\mathrm{msw}}(t) \tag{5-20}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{irr}}(t)$	is the concentration of contaminant j in the irrigation water for lifestyle l [mol/m$^3_{\mathrm{water}}$];
$\mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr,f}}$	is the fraction of irrigation water that is sourced from well for field f and lifestyle l [-] given by Equation (5-30);
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(t)$	is the concentration of contaminant j in the residential well water [mol/m$^3_{\mathrm{water}}$] given by Equation (5-1); and
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{msw}}(t)$	is the main surface water concentration of contaminant j for lifestyle l [mol/m$^3_{\mathrm{water}}$] given by Equation (5-16).

5.2.6 Beach Sediment Concentration

Contaminants can be deposited to beach sediment by wave action, consistent with Clause 7.8.1 of CSA (2020). Thus, the concentration in beach sediment is described with the following equation:

$$\mathrm{C}^{\mathrm{j}}_{\mathrm{sed,beach}}(t) = \mathrm{C}^{\mathrm{j,l}}_{\mathrm{msw}}(t) \cdot \mathrm{P}^{\mathrm{j}}_{\mathrm{wat-sed}} \tag{5-21}$$

where,

$\mathrm{C}^{\mathrm{j}}_{\mathrm{sed,beach}}(t)$	is the concentration of contaminant j in the beach sediment [mol/kg$_{\mathrm{sediment\text{-}dw}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{msw}}(t)$	is the concentration of contaminant j in the main surface waterbody for lifestyle l [mol/kg$_{\mathrm{water}}$] given by Equation (5-16); and
$\mathrm{P}^{\mathrm{j}}_{\mathrm{wat-sed}}$	is the transfer coefficient of dissolved contaminant j in surface water to beach sediments [kg$_{\mathrm{water}}$/kg$_{\mathrm{sediment\text{-}dw}}$] and is defined as the ratio of the concentration in the sediment and the concentration in water in Clause 7.8.1 of CSA (2020).

5.2.7 Groundwater Concentration

The concentration in the groundwater would depend on groundwater discharge and on infiltration from the surface soils. However, for simplicity in the current model, the concentration in the groundwater is assumed to be equivalent to the concentration in the well water. Therefore:

$$\mathrm{C}^{\mathrm{j}}_{\mathrm{groundwater}}(t) = \mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(t) \tag{5-22}$$

where,

$\mathrm{C}^{\mathrm{j}}_{\mathrm{groundwater}}(t)$	is concentration of contaminant j in the groundwater [mol/kg$_{\text{water}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{well,r}}(t)$	is the concentration of contaminant j in the residential well [mol/kg$_{\text{water}}$] given by Equation (5-1).

The groundwater concentration is used for comparison with the chemical hazardous acceptance criteria.

5.2.8 Soil Concentration

Many processes affect the concentration of contaminants in soils. These processes depend on the weather, the soil properties and the depth of the soils. Processes include:

- Terrestrial Discharge – The process by which contaminants are moved from the geosphere into the biosphere via groundwater. Groundwater can enter soils via advection and diffusion and depends on the hydraulic properties of the soils.
- Capillary Rise – is an upward water transport process that is due to water adhesion and surface tension in a porous medium, such as soils and sediments.
- Leaching – the process by which rainfall, snowmelt or irrigation enters the soil through ground surface. Contaminants removed via leaching eventually enter surface waterbodies.
- Erosion – the process by which wind and water movement detach and remove soils (and contaminants) from a field or region.
- Cropping – the process by which soils (and contaminants) are removed via harvesting of crops.
- Irrigation – the process of applying controlled amounts of water to land to assist in the production of crops. Irrigation can introduce contaminants to soils if the source of irrigation water is contaminated or dilute existing contamination in soils if uncontaminated.
- Volatilization – the process by which volatile contaminants are removed from soils and enter the atmosphere.
- Bioturbation – considers the concept that earthworms, burrowing animals and plant roots could bring contaminants up from the subsoil.

Figure 5-2 illustrates the general processes that could influence the concentration of contaminants in the soil.

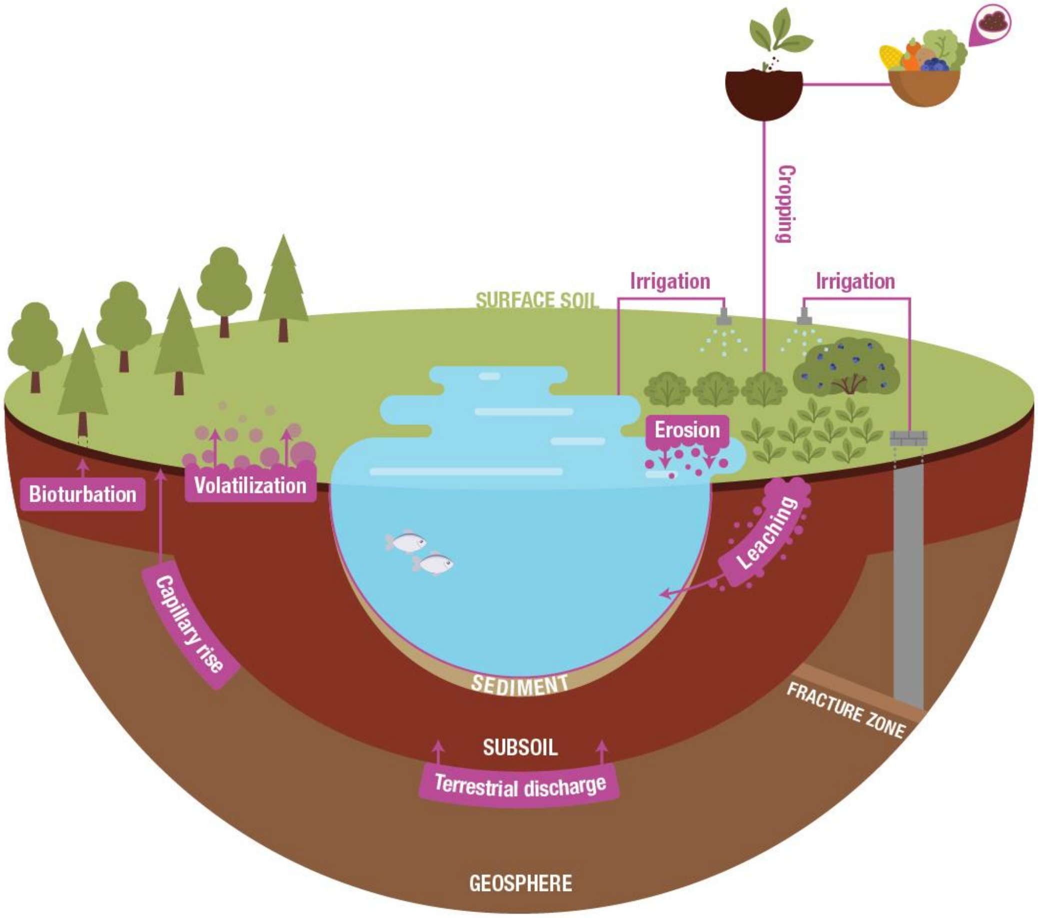

Figure 5-2: Soil Transport Processes

All these processes are depth-limited, meaning the deeper the contamination, the less these processes can bring it to the surface. In the current ISM-BIO model, interactions between the subsoil and surface soils are not modelled. Transfer of contaminants between the two soils are assumed to be instant and from the subsoil to the surface soil. A more detailed modelling of transfer between the subsoil and surface soils will be developed as the site characterization process continues.

For now, it is assumed that all soils are of the same type and experience the same annual precipitation. The irrigation demand per square metre of irrigated soil is then considered to be the same.

5.2.8.1 Soil Sources

There are two routes for contaminants to enter the soil in the ISM-BIO model.

The first is by direct discharge from the geosphere. These release rates are calculated by the geosphere model for specific discharge locations (see Section 4.3.4) and proportional to the field area and geosphere discharge area (see Section 5.2.8.1.1).

The second route is the transfer of contaminants to soils via contaminated irrigation water (see Section 5.2.8.1.2). Deposition is another potential source of contaminants in the soils however this transfer is not included in biosphere model. However, deposition to plants from irrigation water is considered in the dose model (see Section 5.2.12.1).

5.2.8.1.1 Terrestrial Discharge

If a field is not irrigated, the ISM-BIO model assumes that contaminants enter the subsoil from the geosphere model via contaminated groundwater. From the subsoil, contaminants can move up into the surface soils. Two field types (garden and forage field) are considered. Both the garden and the forage fields have areas associated with them (determined in Section 5.2.8.1.1.1 and 5.2.8.1.1.2) as do the terrestrial discharge areas in the geosphere model (see Sections 4.3.4). The geosphere discharge areas are typically much larger than the fields considered in the geosphere area and each field receives discharge proportional the to the field area. In general, the total transport to the soils is given by:

$$\mathrm{X}^{j}_{\mathrm{soil,tot}}(\mathrm{t}) = \left(1-\delta^{l}_{irr,f}\right)\delta^{l}_{msw}\mathrm{f}^{l}_{soil}\mathrm{X}^{j}_{\mathrm{ter,D}}(\mathrm{t}) \tag{5-23}$$

where,

$\mathrm{X}^{j}_{\mathrm{soil,tot}}(\mathrm{t})$	is the total transport from the geosphere to soil for contaminant j [mol/a];
$\mathrm{X}^{j}_{\mathrm{ter,D}}(\mathrm{t})$	is the terrestrial component of the transport from the geosphere model to discharge D [mol/a];
$\delta^{l}_{irr,f}$	is a Boolean parameter that is 1 if the field f is irrigated and 0 if the field is not irrigated;
δ^{l}_{msw}	is a Boolean parameter that is 1 if the surface waterbody is selected by the user to be the main surface waterbody for lifestyle l or 0 if the discharge is not the main surface waterbody; and
$\mathrm{f}^{\mathrm{l}}_{\mathrm{soil}}$	is the fraction of the terrestrial component of the transport from the geosphere entering the garden and forage field soils for lifestyle l defined in Equation (5-24).

The fraction of the terrestrial component of the transport from the geosphere $\mathrm{f}^{\mathrm{l}}_{\mathrm{soil}}$ is given by:

$$\mathrm{f}^{l}_{soil} = \frac{\sum_{f} A^{l}_{f}\left(1-\delta^{l}_{irr,f}\right)}{\sum_{D}\delta^{l}_{msw}A_{D,ter}} \tag{5-24}$$

where,

A^{l}_{f}	is the area of field f for lifestyle l [m^2] given by Equation (5-26) for the garden field and Equation (5-27) for the forage field;
$\delta^{l}_{irr,f}$	is a Boolean parameter that is 1 if the field f is irrigated and 0 if the field is not irrigated;
$A_{D,ter}$	is the area of the terrestrial discharge D in the geosphere model [m^2];
$\delta^{l}_{D,msw}$	is a Boolean parameter that is 1 if the discharge D is selected by the user to be the main surface waterbody for lifestyle l or 0 if the discharge is not the main surface waterbody.

The transport to each field is proportional to the field areas and is given by:

$$\mathrm{X}^{j}_{\mathrm{soil,f}}(\mathrm{t}) = \frac{A^{l}_{f}}{\sum_{f} A^{l}_{f}} \mathrm{X}^{j}_{\mathrm{soil,tot}}(\mathrm{t}) \tag{5-25}$$

where,

$\mathrm{X}^{j}_{\mathrm{soil,f}}(\mathrm{t})$	is the transport from the geosphere to soil in field f for contaminant j [mol/a].

5.2.8.1.1.1 Garden Field Area

The garden is used by some lifestyles to grow vegetables and fruit for consumption. The garden is large enough to supply a lifestyle with the required amount fruits and vegetables. For the purposes of calculating the field area, the model assumes that the ingestion rates of fruits and vegetables correspond to those of the adults[8]. Therefore, the following equation describes the area of the garden field:

$$A^{l}_{garden} = \frac{\mathrm{N}^{l}_{ppl}}{\mathrm{ff}^{l}_{\mathrm{crop,f}}} \sum_{\mathrm{p} \in \mathrm{f}} \frac{\mathrm{R}^{\mathrm{l,a}}_{\mathrm{ing,p}}}{\mathrm{Y}_{\mathrm{p}}} \tag{5-26}$$

where,

A^{l}_{garden}	is the area of the garden field [m^2] for lifestyle l;
N^{l}_{ppl}	is the number of people in the group with a lifestyle [-];
$\mathrm{R}^{\mathrm{l,a}}_{\mathrm{ing,p}}$	is the adult ingestion rate of plant p for lifestyle l [$\mathrm{kg}_{\mathrm{fw}}$/a];
Y_{p}	is the plant yield density for plant p [$\mathrm{kg}_{\mathrm{fw}}/\mathrm{m}^{2}_{\mathrm{soil}}$];
$\mathrm{ff}^{l}_{\mathrm{crop,f}}$	is the cropping frequency of field f and lifestyle l [a^{-1}]; and
$\mathrm{p} \in \mathrm{f}$	refers to the different plants that are grown within the garden field.

5.2.8.1.1.2 Forage Field Area

The forage field has a variety of purposes in the ISM-BIO model. In some lifestyles it is used to grow grain crops such as wheat for consumption by people or livestock. In other lifestyles it contains wild plants and wildlife for consumption by people. In addition, the forage field can also be used for general pasture of livestock and wild game.

The forage field is considered to be large enough to support a lifestyle. For example, in the farmer lifestyle, the forage field is large enough to supply pasture crops for livestock and to grow grains for human (and domestic livestock) consumption. For the purposes of calculating the field area, the model assumes that the ingestion rates correspond to those of the adults. Therefore, the area of the forage fields is calculated as follows:

$$A^{l}_{forage} = \frac{\mathrm{N}^{l}_{ppl}}{\mathrm{ff}^{l}_{\mathrm{crop,f}}} \sum_{\mathrm{p} \in \mathrm{f}} \frac{\mathrm{R}^{\mathrm{l,a}}_{\mathrm{ing,p}}}{\mathrm{Y}_{\mathrm{p}}} + \sum_{\mathrm{ls}} \frac{\mathrm{N}^{l}_{ls}}{\mathrm{ff}^{l}_{\mathrm{crop,f}}} \left(\frac{\mathrm{R}^{\mathrm{l}}_{\mathrm{ing,feed,ls}}}{\mathrm{DW}_{\mathrm{p}} \mathrm{Y}_{\mathrm{feed}}} \right) \tag{5-27}$$

where,

A^{l}_{forage}	is the area of the forage field [m^2];
N^{l}_{ppl}	is the number of people in the lifestyle group [-];

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[8] Note that calculated ingestion doses consider the age group appropriate ingestion rate (see Section 5.2.13.1).

$\mathrm{R}_{\mathrm{ing,p}}^{\mathrm{l,a}}$	is the ingestion rate of plant p for lifestyle l and age group a [$\mathrm{kg_{fw}}$/a];
$\mathrm{Y_p}$	is the plant yield density of plant p [$\mathrm{kg_{fw}/m^2_{soil}}$];
$\mathrm{p} \in \mathrm{f}$	refers to the different plants that are grown within the forage field;
N_{ls}^{l}	is the number of livestock ls for lifestyle l [-] given by Equation (5-28);
$\mathrm{R}_{\mathrm{ing,feed}}^{\mathrm{ls}}$	is the livestock ls ingestion rate of feed for lifestyle l [$\mathrm{kg_{dw}}$/a];
DW_p	is the dry/fresh weight ratio of plant type p used for feed [$\mathrm{kg_{dw}/kg_{fw}}$];
$\mathrm{Y_{feed}}$	is the forage feed yield density [$\mathrm{kg_{fw}/m^2_{soil}}$]; and
$\mathrm{ff}_{\mathrm{crop,f}}^{\mathrm{l}}$	is the cropping frequency of field f [$\mathrm{a^{-1}}$].

The number of livestock of each type (e.g., pigs, cows, chickens) is rounded up to the nearest integer and is calculated as:

$$\mathrm{N}_{ls}^{l} = \frac{\mathrm{N}_{ppl}^{l} \cdot \mathrm{R}_{\mathrm{ing,ls}}^{\mathrm{l,a}}}{\mathrm{Y_{ls}}} \tag{5-28}$$

where,

$\mathrm{N_{ls}}$	is the number of livestock ls for lifestyle l [-];
N_{ppl}^{l}	is the number of people in the lifestyle group [-];
$\mathrm{R}_{\mathrm{ing,ls}}^{\mathrm{l,a}}$	is the ingestion rate of livestock ls for lifestyle l and age group a [$\mathrm{kg_{fw}}$/a]; and
$\mathrm{Y_{ls}}$	is the average dressed yield of livestock ls [$\mathrm{kg_{fw}}$/a].**Irrigation**

Irrigation is the artificial process of applying controlled amounts of water to land to assist in the production of crops. In the ISM-BIO model, irrigation can move contaminants from water sources (i.e., wells and surface waters) to surface soils to increase exposure to humans.

5.2.8.1.2.1 Irrigation from Well Water

Residential well water can be used to irrigate the fields in some lifestyles. The following equation describes the transfer rate:

$$\mathrm{X}_{\mathrm{irr,f}}^{j,\mathrm{l}}(\mathrm{t}) = \mathrm{X}_{\mathrm{well,r}}^{j}(\mathrm{t}) \cdot \frac{\delta_{well,irr,f}^{l} \cdot \mathrm{R}_{\mathrm{irr,f}}^{l}}{\sum_f \mathrm{R}_{\mathrm{irr,f}}^{l}} \cdot \frac{\mathrm{f}_{\mathrm{well,irr}}^{\mathrm{l}} \cdot \mathrm{Q}_{irr}^{l}}{\mathrm{Q}_{well}^{l}} \tag{5-29}$$

where,

$\mathrm{X}_{\mathrm{irr,f}}^{j,\mathrm{l}}(\mathrm{t})$	is the transfer of contaminant j from the well to the field f surface soil [mol/a];
$\mathrm{X}_{\mathrm{well,r}}^{\mathrm{j}}(t)$	is the discharge rate of contaminant j from geosphere to the residential well [mol/a];
$\mathrm{R}_{\mathrm{irr,f}}^{\mathrm{l}}$	is the irrigation rate of field f for lifestyle l [$\mathrm{m^3_{water}/a/m^2_{soil}}$];
$\mathrm{f}_{\mathrm{well,irr}}^{\mathrm{l}}$	is the fraction irrigation water that is sourced from the well for field f and lifestyle l [-] given by Equation (5-30);
Q_{well}^{l}	is the total well demand [$\mathrm{m^3_{water}}$/a] for lifestyle l;
Q_{irr}^{l}	is the irrigation water demand [$\mathrm{m^3_{water}}$/a] for lifestyle l as defined in Equation (5-5); and
$\delta_{well,irr,f}^{l}$	is a Boolean parameter that is 1 if the well is used to irrigate field f

in lifestyle l and 0 if a different source of water is used to irrigate field f or if fields are not irrigated in lifestyle l.

The fraction irrigation water that is taken from the well if given by:

$$\mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr}} = \begin{cases} 1 & \text{If } \mathrm{Q}^{l}_{cap} \geq \mathrm{Q}^{l}_{dom} + \mathrm{Q}^{l}_{ls} + \mathrm{Q}^{l}_{irr} \text{ and } \delta^{l}_{irr,f} = 1 \\ (\mathrm{Q}_{\mathrm{cap}} - \mathrm{Q}^{l}_{dom} - \mathrm{Q}^{l}_{ls})/\mathrm{Q}_{\mathrm{irr}} & \text{If } \mathrm{Q}^{l}_{dom} + \mathrm{Q}^{l}_{irr} < \mathrm{Q}^{l}_{cap} < \mathrm{Q}^{l}_{dom} + \mathrm{Q}^{l}_{ls} + \mathrm{Q}^{l}_{irr} \\ & \text{and } \mathrm{Q}^{l}_{irr} > 0 \\ 0 & \text{If } \mathrm{Q}^{l}_{cap} \leq \mathrm{Q}^{l}_{dom} + \mathrm{Q}^{l}_{ls} \text{ or } \mathrm{Q}^{l}_{irr} = 0 \end{cases} \tag{5-30}$$

where,

$\mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr}}$	is the fraction irrigation water that is sourced from the well for lifestyle l [-];
Q^{l}_{cap}	is the annual well capacity $[\mathrm{m}^3_{\mathrm{water}}/\mathrm{a}]$ for lifestyle l;
Q^{l}_{dom}	is the domestic water demand $[\mathrm{m}^3_{\mathrm{water}}/\mathrm{a}]$ for lifestyle l;
Q^{l}_{ls}	is the livestock water demand $[\mathrm{m}^3_{\mathrm{water}}/\mathrm{a}]$ for lifestyle l; and
Q^{l}_{irr}	is the irrigation water demand $[\mathrm{m}^3_{\mathrm{water}}/\mathrm{a}]$;

5.2.8.1.2.2 Irrigation from Surface Water

For lifestyles where the main surface waterbody is used as the primary source of irrigation water or if a well is used and supplemented with surface water, the rate of transfer from surface water features to fields through irrigation is given by:

$$\lambda^{\mathrm{j,l}}_{\mathrm{irr,f}}(\mathrm{t}) = \frac{\mathrm{N}^{\mathrm{j}}_{\mathrm{msw}}(\mathrm{t}) \cdot \mathrm{R}^{\mathrm{l}}_{\mathrm{irr,f}} \cdot \mathrm{A}^{l}_{f} \cdot \left(1 - \delta^{l}_{well,irr,f} \cdot \mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr}}\right)}{\mathrm{V}^{l}_{msw}} \tag{5-31}$$

where,

$\lambda^{\mathrm{j,l}}_{\mathrm{irr,f}}(\mathrm{t})$	is the irrigation transfer rate from the main surface waterbody to the soil of field f for lifestyle l and contaminant j [mol/a];
$N^{j}_{msw}(t)$	is the amount of contaminant j in the main surface waterbody (compartment) as determined by the biosphere model [mol];
$\mathrm{R}^{\mathrm{l}}_{\mathrm{irr,f}}$	is the irrigation rate of field f for lifestyle l $[\mathrm{m}^3_{\mathrm{water}}/\mathrm{a}/\mathrm{m}^2_{\mathrm{soil}}]$;
A^{l}_{f}	is the area of field f for lifestyle l $[\mathrm{m}^2_{\mathrm{soil}}]$;
V^{l}_{msw}	is the volume of the main surface waterbody for lifestyle l $[\mathrm{m}^3_{\mathrm{water}}]$;
$\mathrm{f}^{\mathrm{l}}_{\mathrm{well,irr,f}}$	is the fraction of irrigation water sourced from the well for field f and lifestyle l [-] defined in Equation (5-30); and
$\delta^{l}_{well,irr,f}$	is a Boolean parameter that is 1 if the well is used to irrigate field f in lifestyle l or 0 if a different source of water is used to irrigate field f or if fields are not irrigated in lifestyle l.

5.2.8.2 Soil Losses

There are four loss terms for the soil compartments. These include leaching (Section 5.2.8.2.1), erosion (Section 5.2.8.2.2), cropping (Section 5.2.8.2.3), and volatilization (Section 5.2.8.2.4).

5.2.8.2.1 Leaching

Leaching is the downward movement of contaminants into the soil by infiltrating water. The contaminants are lost from the surface soil but are assumed to quickly move down to the water table and from there into the main surface waterbody. Clause 6.3.6.1 of CSA (2020) recommends the following equation for the leaching rate:

$$\lambda^{j}_{\mathrm{leach,f}}(t) = \frac{N^{j}_{f}(t) \cdot q_{\mathrm{infil}} \cdot f^{j}_{\mathrm{wat}}}{\theta_{w} \cdot Z_{s}} \tag{5-32}$$

where,

$\lambda^{j}_{\mathrm{leach,f}}(t)$	is the leaching rate of contaminant j from field f [mol/a];
$N^{j}_{f}(t)$	is the amount of contaminant j in surface soil (compartment) for field f as determined by the biosphere model [mol];
q_{infil}	is the net infiltration rate of water through the soil [$m^3/m^2/a$] given by Equation (5-34);
Z_s	is the depth of the surface soil layer [m];
θ_w	is the soil water content [$m^3_{\mathrm{water}}/m^3_{\mathrm{soil}}$]; and
f^{j}_{wat}	is the fraction of contaminant j in soil in the water phase (i.e., not sorbed), which is given by Equation (5-33):

$$f^{j}_{\mathrm{wat}} = \frac{\theta_{w}}{\theta_{w} + kd^{j}_{\mathrm{soil}} \cdot \rho_{\mathrm{soil}}} \tag{5-33}$$

where,

θ_w	is the soil water content [$m^3_{\mathrm{water}}/m^3_{\mathrm{soil}}$];
kd^{j}_{soil}	is the solid-to-liquid partition coefficient for soil for contaminant j [$m^3_{\mathrm{water}}/kg_{\mathrm{soil\text{-}dw}}$];
ρ_{soil}	is the soil density [$kg_{\mathrm{soil\text{-}dw}} / m^3_{\mathrm{soil}}$].

CSA (2020) assumes that irrigation is only applied to wet the top 5-10 cm of soil to field capacity, meaning little or none of the irrigation water applied would pass below the surface layer. The net infiltration rate of water through soil is therefore the balance between precipitation, surface runoff and evapotranspiration. It is assumed to equal half the difference between the annual precipitation and the runoff (Clause 6.3.6.2 of CSA 2020), thus:

$$q_{\mathrm{infil}} = \frac{P_{\mathrm{tot}} - R_{T}}{2} \text{ (if } P_{\mathrm{tot}} > R_{T}\text{, otherwise 0)} \tag{5-34}$$

where,

q_{infil}	is the net infiltration rate of water through the soil [$m^3_{\mathrm{water}}/(m^2_{\mathrm{soil}}\ a)$];
P_{tot}	is the total precipitation rate [$m^3_{\mathrm{water}}/(m^2_{\mathrm{soil}}\ a)$]; and
R_T	is the average watershed runoff [$m^3_{\mathrm{water}}/(m^2_{\mathrm{soil}}\ a)$].

5.2.8.2.2 Erosion

Erosion of the surface soil is characterized by a soil erosion rate constant and contaminants lost from the soil via erosion are assumed to be transferred to the main surface waterbody. The associated erosive transfer rate from the soil is defined in Clause 6.3.4.1 of CSA (2020) and is given by:

$$\lambda^{j}_{er,f}(\mathrm{t}) = \frac{\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t}) \cdot \mathrm{ER} \cdot (1 - \mathrm{f}_{\mathrm{wat}})}{\rho_{\mathrm{soil}} \cdot \mathrm{Z}_{\mathrm{s}}} \tag{5-35}$$

where,

$\lambda^{j}_{er,f}(\mathrm{t})$	is the erosive rate of contaminant j from field f [1/a];
$\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t})$	is the amount of contaminant j in surface soil (compartment) for field f as determined by the biosphere model [mol];
ER	is the erosion rate [$\mathrm{kg_{dw}/m^2{}_{soil}/a}$];
ρ_{soil}	is the soil density [$\mathrm{kg_{dw}/m^3{}_{soil}}$]; and
$\mathrm{Z_s}$	is the depth of the active surface soil layer [$\mathrm{m_{soil}}$].

5.2.8.2.3 Cropping

Contaminants can be lost from the surface soils due to the cropping cycle. This process is described as a loss from the system (i.e., transfer to the sink). A low cropping rate is conservative for the purpose of assessing consequences of soil exposure. The cropping loss is defined in Clause 6.3.7.1 of CSA (2020) and is given by:

$$\lambda^{\mathrm{j,l}}_{\mathrm{crop,f}}(\mathrm{t}) = \frac{\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t}) \cdot \mathrm{f_c} \cdot \mathrm{ff}^{l}_{\mathrm{crop,f}}}{\mathrm{Z_s} \cdot \rho_{\mathrm{soil}}} \cdot \ \mathrm{min}_{\mathrm{p \in f}}\left(\frac{\mathrm{CR_p} \cdot \mathrm{Y_{f,p}}}{\mathrm{HI}}\right) \tag{5-36}$$

where,

$\lambda^{\mathrm{j,l}}_{\mathrm{crop,f}}(t)$	is the cropping loss rate of contaminant j for field f and lifestyle l [mol/a];
$\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t})$	is the amount of contaminant j in surface soil (compartment) for field f as determined by the biosphere model [mol];
$\mathrm{f_c}$	is the fraction of crop elemental composition lost each year [-];
$\mathrm{ff}^{\mathrm{l}}_{\mathrm{crop,f}}$	is the cropping frequency of field f for lifestyle l [1/a];
$\mathrm{Z_s}$	is the thickness of the active soil layer [$\mathrm{m_{soil}}$];
ρ_{soil}	is the soil density [$\mathrm{kg_{soil\text{-}dw}/m^3{}_{soil}}$];
$\mathrm{p \in f}$	refers to the plants p that are in field f (i.e., fruits and vegetables in the garden field, grains and forage crops in the forage field);
$\mathrm{CR^j_p}$	is the plant/soil concentration ratio for contaminant j and plant p [$\mathrm{kg_{soil\text{-}dw}/kg_{plant\text{-}fw}}$];
$\mathrm{Y_{f,p}}$	is the plant yield density for field type f and plant p [$\mathrm{kg_{plant\text{-}fw}/m^2{}_{soil}}$]; and
HI	is the harvest index (mass of consumable product divided by mass of total above-ground plant (total below-ground plant for root crops).

5.2.8.2.4 Volatilization

Contaminants can enter the atmosphere from soil via volatilization. This process is described as a loss from the system (i.e., transfer to the sink), not as a transfer to an air compartment. Loss from the soil is modelled assuming a soil volatilization rate constant and the loss rate from a given field is given by:

$$\lambda^{j}_{vol,f}(\mathrm{t}) = \mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t}) \cdot \mathrm{VR}^{j}_{soil} \tag{5-37}$$

where,

$\lambda^{j}_{vol,f}(\mathrm{t})$	is the loss rate of contaminant j from a field due to volatilization [mol/a];
$\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(\mathrm{t})$	is the amount of contaminant j in the soil (compartment) for field f, as determined by the biosphere model [mol]; and
VR^{j}_{soil}	is the soil volatilization rate constant for contaminant j [1/a].

5.2.9 Surface Soil Concentration

The concentration of contaminant is calculated from the amount of contaminant in the soil compartment. The amount of contaminant is calculated by AMBER numerically as the sum of sources, inflows and subtraction of outflows and decay. The equation applied in amber is:

$$\begin{aligned}\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(t) = \mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(t^{-1}) \\ + \Delta\mathrm{t}\Big[\mathrm{X}^{j}_{\mathrm{soil,tot}}(t^{-1}) - \lambda^{j}_{er,f}(t^{-1}) - \lambda^{\mathrm{j}}_{\mathrm{leach,f}}(t^{-1}) - \lambda^{\mathrm{j,l}}_{\mathrm{crop,f}}(t^{-1}) \\ - \lambda^{j}_{vol,f}(t^{-1}) - \lambda^{j}_{dec}\mathrm{N}^{\mathrm{j}}_{w}(t^{-1})\Big]\end{aligned} \tag{5-38}$$

where,

$\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(t)$	is the amount of contaminant j in the field soil f(compartment) as determined by the biosphere model [mol];
$\mathrm{X}^{j}_{\mathrm{soil,tot}}$	is the total transport from the geosphere to soil for contaminant j [mol/a];
$\mathrm{X}^{j,\mathrm{l}}_{\mathrm{irr,f}}$	is the transfer of contaminant j from the well to the field f surface soil [mol/a];
$\lambda^{\mathrm{j}}_{\mathrm{leach,f}}$	is the leaching rate of contaminant j from field f [mol/a];
$\lambda^{j}_{er,f}$	is the erosive rate of contaminant j from field f [mol/a];
$\lambda^{\mathrm{j,l}}_{\mathrm{crop,f}}$	is the cropping loss rate of contaminant j for field f and lifestyle l [mol/a];
$\lambda^{j}_{vol,f}$	is the loss rate of contaminant j from a field due to volatilization [mol/a];

The contaminant j concentration in surface soil for the garden and forage field [mol/kg] is given by the following equation:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{soil,f}}(\mathrm{t}) = (1-\delta_{wetland})\frac{\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(t)}{A^{l}_{f}\cdot\mathrm{Z_s}\cdot\rho_{\mathrm{soil}}} + \delta_{wetland}\,max_{w}\big(C^{j}_{sed,wetland,w}(t)\big) \tag{5-39}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{soil,f}}(t)$	is the concentration of contaminant j in the soil in the field f for lifestyle l [mol/kg$_{\mathrm{soil}}$];
$\mathrm{N}^{\mathrm{j}}_{\mathrm{f}}(t)$	is the amount of contaminant j in the field soil f(compartment) as determined by the biosphere model [mol];
A^{l}_{f}	is the area of field f for lifestyle l [m$^2_{\mathrm{soil}}$] given by Equation (5-26) and Equation (5-27);
$\mathrm{Z_s}$	is the thickness of the surface soil layer [m$_{\mathrm{soil}}$];
ρ_{soil}	is the soil density [kg$_{\mathrm{dw}}$/m$^3_{\mathrm{soil}}$];
$\delta_{wetland}$	is a Boolean parameter that is 1 if a wetland is assumed converted to fields (garden and forage) and zero otherwise; and
$C^{j}_{sed,wetland,w}(t)$	is the concentration of contaminant j in wetland w sediment [mol/kg$_{\mathrm{sediment}}$] given by Equation (5-47); and

λ_{dec}^{j} is the decay constant of contaminant j [1/a].

5.2.10 Wetlands Organic Sediment Concentration

Contaminants are discharged from the geosphere to one or more wetlands through terrestrial discharge. The geosphere model determines the amounts of contaminant discharged to each wetland (see Section 4.3.4). The transport processes included in the model are illustrated in Figure 5-3.

The transfers to and from the plants, humans, and animals are all not expected to result in any significant net input or output of contaminants within the wetland. Furthermore, these processes are typically associated with time constants much smaller than those relevant to post-closure safety analyses. Consequently, they are not considered. The current model considers minimal release of contaminant to the airshed; therefore, deposition to wetland organic sediments is not considered.

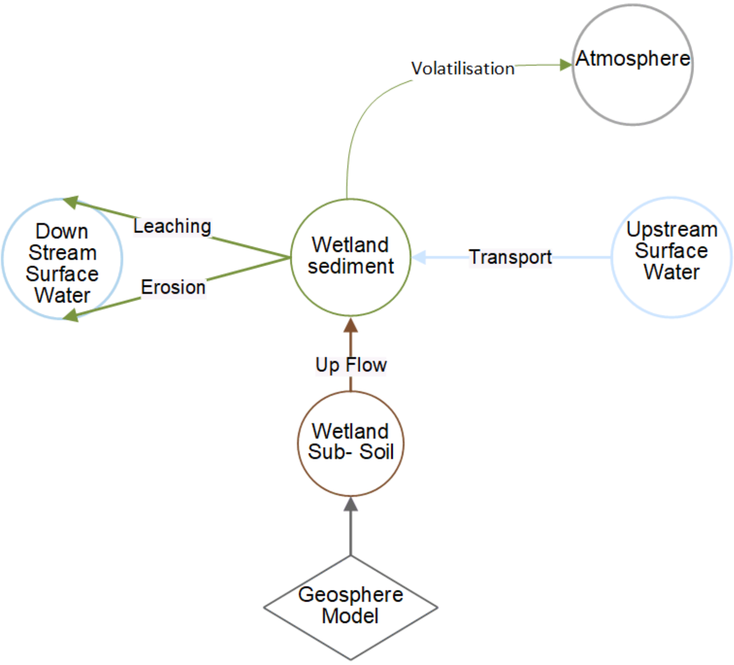

Figure 5-3: Wetland Conceptual Model

5.2.10.1 Wetlands Organic Sediment Sources

Contaminants can enter wetlands via direct discharge from the geosphere and inflow from upstream wetlands or surface water features (see Figure 5-3).

5.2.10.1.1 Discharge to Wetlands

Contaminants can enter wetlands in the biosphere model directly from the geosphere model. Discharge to wetlands is calculated by the geosphere model (see Section 4.3.4), specifically:

$$\mathrm{X}^{j}_{\mathrm{wetland}}(\mathrm{t}) = \mathrm{X}^{j}_{\mathrm{D}}(\mathrm{t}) \qquad (5\text{-}40)$$

where,

$\mathrm{X}^{j}_{\mathrm{wetland}}(\mathrm{t})$ is the transport from the geosphere to wetland w for contaminant j [mol/a]; and
$\mathrm{X}^{j}_{\mathrm{D}}(\mathrm{t})$ is the transport from the geosphere model to discharge D [mol/a];

5.2.10.1.2 Inflow from Upstream Surface Water Features

The rate at which contaminants are transferred from an upstream surface water features (e.g., lakes, rivers, other wetlands) to a downstream feature is described by Equation (5-9).

5.2.10.2 Wetlands Organic Sediment Losses

Losses from wetlands included in the biosphere model are loss to a downstream surface water feature through erosion and leaching, and loss to a sink via volatilization.

5.2.10.2.1 Leaching

Leaching is the movement of contaminants through the wetland sediment by discharging water. The contaminants are lost from the wetland sediment but are assumed to discharge to the downstream surface water feature. The wetland leaching equation was adapted from the soil leaching equation in clause 6.3.6.1 of CSA (2020) and is given by:

$$\lambda^{\mathrm{j}}_{\mathrm{leach,w}}(\mathrm{t}) = \frac{\mathrm{N}^{\mathrm{j}}_{w}(\mathrm{t}) \cdot q_{\mathrm{w}} \cdot \mathrm{f}^{\mathrm{j}}_{\mathrm{w}}}{\theta_{ws} \cdot Z_{w}} \qquad (5\text{-}41)$$

where,

$\lambda^{\mathrm{j}}_{\mathrm{leach,w}}(\mathrm{t})$ is the leaching rate of contaminant j from wetland w [mol/a];
$\mathrm{N}^{j}_{w}(\mathrm{t})$ is the amount of contaminant j in wetland sediment (compartment w) as determined by the biosphere model [mol];
q_{w} is the flux of water through the wetland [m/a] given by Equation (5-43);
Z_{w} is the depth of the wetland sediment [m];
θ_{ws} is the wetland sediment water content [$\mathrm{m^3_{water}/m^3_{wetland}}$]; and
$\mathrm{f}^{\mathrm{j}}_{\mathrm{w}}$ is the fraction of contaminant j in wetland sediment in the water phase (i.e., not sorbed), which is given by Equation (5-42):

$$\mathrm{f}^{\mathrm{j}}_{\mathrm{w}} = \frac{\theta_{\mathrm{ws}}}{\theta_{\mathrm{ws}} + \mathrm{kd}^{\mathrm{j}}_{w} \cdot \rho_{\mathrm{w}}} \qquad (5\text{-}42)$$

where,

θ_{ws} is the wetland sediment water content [$\mathrm{m^3_{water}/m^3_{soil}}$];
$\mathrm{kd}^{\mathrm{j}}_{\mathrm{w}}$ is the solid-to-liquid partition coefficient for wetland sediment for contaminant j [$\mathrm{m^3_{water}/kg_{wetland\text{-}dw}}$];
ρ_{w} is the wetland sediment density [$\mathrm{kg_{wetland\text{-}dw} / m^3_{soil}}$].

$$\mathrm{q_w} = \frac{\mathrm{Qw}}{\mathrm{Aw}} \qquad (5\text{-}43)$$

where,

$\mathrm{q_w}$ is the net infiltration rate of water through the soil [$\mathrm{m^3}$ water /($\mathrm{m^2}$ wetland a)];
$\mathrm{A_w}$ is the area of the wetland [$\mathrm{m^2}$wetland]; and
$\mathrm{Q_w}$ is the total water flow through the wetland [$\mathrm{m^3}$ water /a)].

5.2.10.2.2 Erosion

Erosion of the wetland sediment is characterized by a wetland erosion rate constant and contaminants lost from the wetland via erosion are assumed to be transferred to the downstream surface water feature. The wetland erosion equation was adapted from the soil leaching equation in clause 6.3.4.1 of CSA (2020) and is given by:

$$\lambda_{er,w}^{j}(\mathrm{t}) = \frac{\mathrm{N}_{w}^{\mathrm{j}}(\mathrm{t}) \cdot \mathrm{ER}_{w} \cdot (1 - \mathrm{f}_{\mathrm{w}}^{\mathrm{j}})}{\rho_{\mathrm{w}} \cdot \mathrm{Z_w}} \tag{5-44}$$

where,

$\lambda_{er,w}^{j}(\mathrm{t})$	is the erosive rate of contaminant j from wetland w [mol/a];
$\mathrm{N}_{w}^{\mathrm{j}}(\mathrm{t})$	is the amount of contaminant j in wetland sediment (compartment) for wetland w as determined by the biosphere model [mol];
ER_{w}	is the erosion rate from the wetland [$\mathrm{kg_{dw}/m^2}$ wetland/a];
ρ_{w}	is the wetland sediment density [$\mathrm{kg_{dw}/m^3}$ wetland];
Z_{w}	is the depth of the wetland sediment [m]; and
$\mathrm{f}_{\mathrm{w}}^{\mathrm{j}}$	is the fraction of contaminant j in wetland sediment in the water phase (i.e., not sorbed), which is given by Equation (5-42).

5.2.10.2.3 Volatilization

Contaminants can leave the wetland and enter the atmosphere via volatilization. This process is described as a loss from the system (i.e., transfer to the sink), not as a transfer to an air compartment. Loss from the wetland sediment is modelled assuming a soil volatilization rate constant and the loss rate from a given wetland is given by:

$$\lambda_{vol,w}^{j}(\mathrm{t}) = \mathrm{N}_{w}^{\mathrm{j}}(\mathrm{t}) \cdot \mathrm{VR}_{wetland}^{j} \tag{5-45}$$

where,

$\lambda_{vol,w}^{j}(\mathrm{t})$	is the loss rate of contaminant j from a wetland, w, due to volatilization [mol/a];
$\mathrm{N}_{w}^{\mathrm{j}}(\mathrm{t})$	is the amount of contaminant j in wetland sediment (compartment) for wetland w as determined by the biosphere model [mol];
$\mathrm{VR}_{wetland}^{j}$	is the wetland volatilization rate constant for contaminant j [1/a].

5.2.10.3 Wetlands Organic Sediment Concentration

The concentration of contaminant is calculated from the amount of contaminant in the soil compartment. The amount of contaminant is calculated by AMBER numerically as the sum of sources, inflows and subtraction of outflows and decay. The equation applied in amber is:

$$\mathrm{N}^{\mathrm{j}}_{w}(t) = \mathrm{N}^{\mathrm{j}}_{w}(t^{-1}) + \Delta \mathrm{t}\left[\mathrm{X}^{j}_{\mathrm{wetland}}(t^{-1}) + \left(\sum_{up\ sw} \lambda^{j}_{inflow,sw}(t^{-1})\right) - \lambda^{j}_{er,w}(t^{-1}) - \lambda^{\mathrm{j}}_{\mathrm{leach,w}}(t^{-1}) - \lambda^{j}_{vol,w}(t^{-1}) - \lambda^{j}_{dec}\mathrm{N}^{\mathrm{j}}_{w}(t^{-1})\right] \tag{5-46}$$

where,

$\mathrm{N}^{\mathrm{j}}_{w}$	is the amount of contaminant j in the wetland w (compartment) as determined by the biosphere model [mol];
$\mathrm{X}^{j}_{\mathrm{wetland}}$	is the transport from the geosphere to wetland w for contaminant j [mol/a];
$\mathrm{X}^{j,\mathrm{l}}_{\mathrm{irr,f}}(\mathrm{t})$	is the transfer of contaminant j from the well to the field f surface soil [mol/a];
$\lambda^{j}_{inflow,sw}$	is the transfer rate of contaminant j from the upstream surface water feature to the wetland [mol/a];
$\lambda^{\mathrm{j}}_{\mathrm{leach,w}}$	is the leaching rate of contaminant j from wetland w [mol/a];
$\lambda^{j}_{er,w}$	is the erosive rate of contaminant j from wetland w [mol/a];
$\lambda^{j}_{vol,w}$	is the loss rate of contaminant j from a wetland, w, due to volatilization [mol/a]; and
λ^{j}_{dec}	is the decay constant of contaminant j [1/a].

The contaminant j concentration in wetland organic sediment for each wetland w [mol/kg] is given by the following equation:

$$\mathrm{C}^{\mathrm{j}}_{sed,wetland,w}(\mathrm{t}) = \frac{\mathrm{N}^{\mathrm{j}}_{w}(t)}{\mathrm{A_w} \cdot \mathrm{Z_w} \cdot \rho_{\mathrm{w}}} \tag{5-47}$$

where,

$\mathrm{C}^{\mathrm{j}}_{\mathrm{sed,wetland,w}}(t)$	is the concentration of contaminant j in wetland w sediment [$\mathrm{mol/kg_{sediment}}$];
$\mathrm{N}^{\mathrm{j}}_{w}(t)$	is the amount of contaminant j in the wetland w (compartment) as determined by the biosphere model [mol];
$\mathrm{A_w}$	is the area of the wetland [$\mathrm{m^2_{wetland}}$];
$\mathrm{Z_w}$	is the thickness of the wetland sediment [$\mathrm{m_{wetland}}$]; and
ρ_{w}	is the wetland sediment density [$\mathrm{kg_{dw}/m^3\,_{wetland}}$].

5.2.11 Air Concentration

The following sections describe the outdoor and indoor air concentration in the biosphere model. Figure 5-4 illustrates the air transport processes that influence the concentration of contaminants in the indoor and outdoor air in the ISM-BIO models.

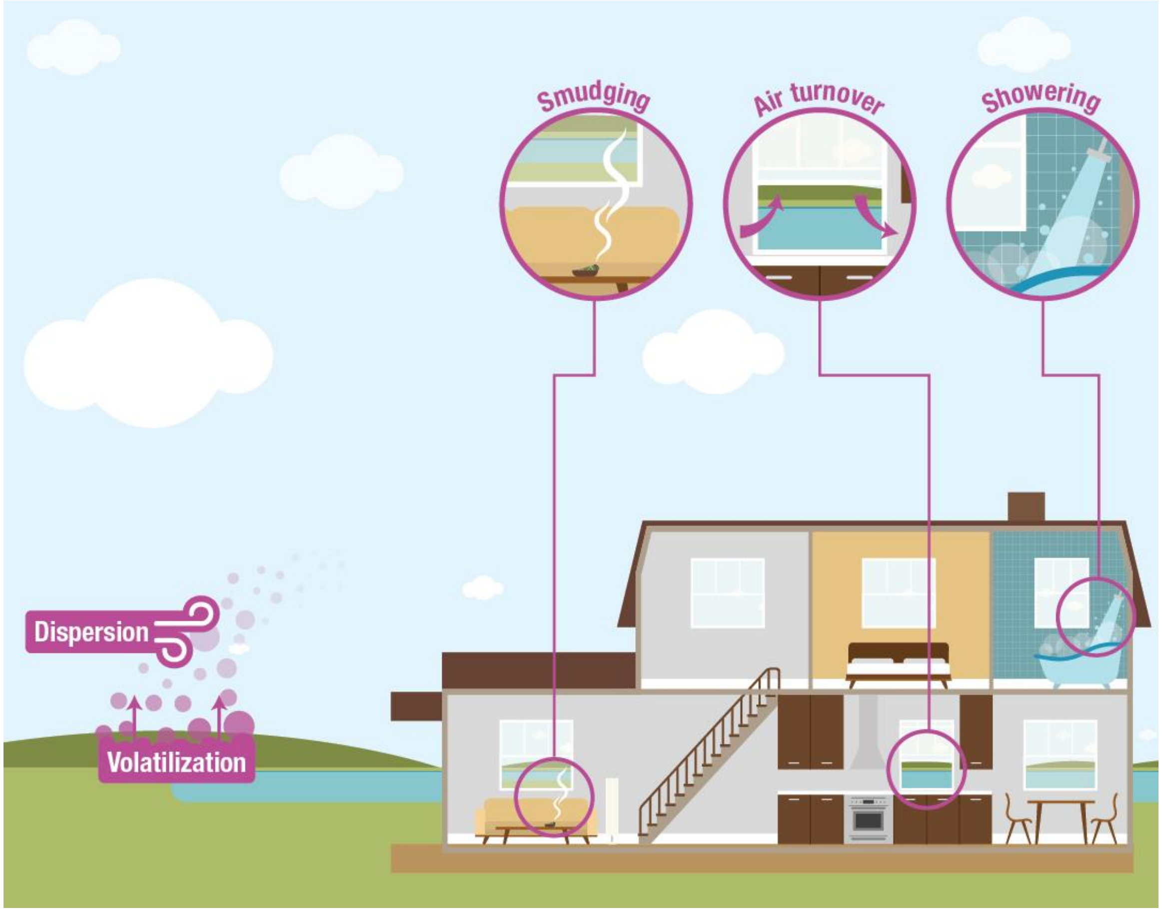

Figure 5-4: Air Pathways

5.2.11.1 Outdoor Air Concentration

CSA (2020) provides guidance on modelling airborne concentration from effluent releases from facilities. However, because of the nature of the releases from an underground repository, only a small number of the equations describing atmosphere concentration in CSA (2020) can be used in the ISM-BIO model.

As per the CSA (2020), the outdoor air concentration is modelled as an equilibrium process. In general, contaminants can enter the atmosphere from soils and surface waters via volatilization. In the biosphere model, the exposures to humans and non-human biota assumes the maximum outdoor air concentration across all field and surface waterbodies. Implicit in this approach is the assumption that the atmosphere above the fields and surface waters do not mix. The concentration in air above the soil is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,f}}(\mathrm{t}) = \mathrm{P}^{\mathrm{j}}_{\mathrm{soil-air,f}}\mathrm{C}^{\mathrm{j,l}}_{\mathrm{soil,f}}(t) \tag{5-48}$$

where,

$C^{j,l}_{\mathrm{air,outdoor,f}}(t)$	is the outdoor air concentration above field f for lifestyle l [mol/$\mathrm{m^3_{air}}$];
$P^{j}_{\mathrm{soil-air,f}}$	is the transfer parameter from irrigated soil to air for field f and contaminant j [$\mathrm{kg_{soil}}$/$\mathrm{m^3_{air}}$] described by Equation (5-49); and
$C^{j,l}_{\mathrm{soil,f}}(t)$	is the concentration of contaminant j in the soil in field f for lifestyle l [mol/$\mathrm{kg_{soil}}$] described by Equation (5-39).

The equilibrium factor describing the concentration in air from volatilization from soil is (Clause 7.2.5.1 of CSA 2020):

$$P^{j}_{\mathrm{soil-air,f}} = (1-\delta_{wetland})\cdot \mathrm{Z_{soil}}\cdot \rho_{\mathrm{soil}}\cdot VR^{j}_{\mathrm{soil}}\cdot \mathrm{D_{res,f}}\cdot \mathrm{C_{res}} + \delta_{wetland}\cdot \max(\mathrm{Z_w}) \cdot \rho_{\mathrm{w}}\cdot VR^{j}_{\mathrm{wetland}}\cdot \max(\mathrm{D_{res,w}}\cdot \mathrm{C_{res}}) \tag{5-49}$$

where,

$P^{j}_{\mathrm{soil-air,f}}$	is the transfer parameter from irrigated soil to air for field f and contaminant j [$\mathrm{kg_{soil}}$/$\mathrm{m^3_{air}}$];
Z_{soil}	is the depth of the surface soil [$\mathrm{m_{soil}}$];
ρ_{soil}	is the soil density [$\mathrm{kg_{soil\text{-}dw}}$/$\mathrm{m^3_{soil}}$];
$\mathrm{VR}^{j}_{\mathrm{soil}}$	is the terrestrial volatilization rate constant for contaminant j [1/a];
$D_{res,f}$	is the air dilution factor for terrestrial volatilization in field f [a $\mathrm{m^2_{soil}}$/$\mathrm{m^3_{air}}$] described by Equation (5-50);
C_{res}	is a correction factor that accounts for the location of the receptor relative to the field [-]. This is assumed to be the conservative default value of 1 in the ISM-BIO model as per Clause 7.2.5.3 of CSA (2020).
$\delta_{wetland}$	is a Boolean parameter that is 1 if a wetland is assumed converted to fields (garden and forage) and zero otherwise;
Z_w	is the depth of the wetland sediment [$\mathrm{w_{etland\ sediment}}$];
ρ_{w}	is the wetland sediment density [$\mathrm{kg_{wetland\text{-}dw}}$ / $\mathrm{m^3_{soil}}$].
$\mathrm{VR}^{j}_{wetland}$	is the wetland volatilization rate constant for contaminant j [1/a]; and
$D_{res,w}$	is the air dilution factor for terrestrial volatilization in wetland w [a $\mathrm{m^2_{soil}}$/$\mathrm{m^3_{air}}$] described by Equation (5-50);

The air dilution factor for terrestrial volatilization [a/m] accounts for dispersion in air from the source to the receptor. It is given by Clause 7.2.5.2 of CSA (2020):

$$D_{res,f} = \left(4.87 {A_f^{l}}^{\frac{1}{8}} - 3.56\right)\cdot f_{s-a} \tag{5-50}$$

$D_{res,f}$	is the air dilution factor for terrestrial volatilization [(a $\mathrm{m^2_{soil}}$)/$\mathrm{m^3_{air}}$];
A_f^l	is the area of field f in lifestyle l [$\mathrm{m^2}$]; and
f_{s-a}	is the conversion factor from seconds to years [a/s].

$$D_{res,w} = \left(4.87 {A_w}^{\frac{1}{8}} - 3.56\right)\cdot f_{s-a} \tag{5-51}$$

$D_{res,w}$	is the air dilution factor for terrestrial volatilization from a wetland [(a $\mathrm{m^2_{soil}}$)/$\mathrm{m^3_{air}}$];
A_w	is the area of the wetland w [$\mathrm{m^2}$]; and
f_{s-a}	is the conversion factor from seconds to years [a/s].

The concentration in air above the surface water is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,sw}}(\mathrm{t}) = \mathrm{P}^{\mathrm{j}}_{\mathrm{sw-air,sw}} \mathrm{C}^{\mathrm{j,l}}_{\mathrm{sw}}(t) \tag{5-52}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,sw}}(t)$	is the outdoor air concentration above surface water feature sw for lifestyle l [mol/$\mathrm{m^3_{air}}$];
$\mathrm{P}^{\mathrm{j}}_{\mathrm{sw-air,sw}}$	is the transfer parameter from surface water to air for surface water feature sw and contaminant j [$\mathrm{kg_{water}}$/$\mathrm{m^3_{air}}$] described by Equation (5-53);
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{sw}}(t)$	is the concentration of contaminant j in the surface water feature sw for lifestyle l [mol/$\mathrm{kg_{water}}$] described by Equation (5-15);

The equilibrium factor describing the concentration in air from volatilization from surface waters is as follows (based on Clause 7.2.5.1 of CSA 2020):

$$\mathrm{P}^{\mathrm{j}}_{\mathrm{sw-air,sw}} = \mathrm{Z}_{\mathrm{sw}} \cdot \rho_{\mathrm{wat}} \cdot VR^{j}_{wat} \cdot \mathrm{D}_{\mathrm{res,sw}} \tag{5-53}$$

where,

$\mathrm{P}^{\mathrm{j}}_{\mathrm{air-sw,sw}}$	is the transfer parameter from surface water to air for surface water feature sw and contaminant j [$\mathrm{kg_{water}}$/$\mathrm{m^3_{air}}$];
Z_{sw}	is the depth of the surface water feature sw [$\mathrm{m_{water}}$];
ρ_{wat}	is the water density [$\mathrm{kg_{water}}$/$\mathrm{m^3_{water}}$];
$\mathrm{VR}^{j}_{\mathrm{wat}}$	is the water volatilization rate constant for contaminant j [1/a]; and
$D_{res,sw}$	is the air dilution factor for aquatic volatilization [a $\mathrm{m^2_{water}}$/$\mathrm{m^3_{air}}$] described by Equation (5-54).

The air dilution factor for aquatic volatilization [a/m] accounts for dispersion in air from the source to the receptor. It is given by Clause 7.2.5.2 of CSA (2020):

$$D_{res,sw} = \left(4.87 {A_{sw}}^{\frac{1}{8}} - 3.56\right) \cdot f_{s-a} \tag{5-54}$$

$D_{res,sw}$	is the air dilution factor for terrestrial volatilization [(a $\mathrm{m^2_{water}}$)/$\mathrm{m^3_{air}}$];
A_{sw}	is the area of surface water feature sw [$\mathrm{m^2_{water}}$]; and
f_{s-a}	is the conversion factor from seconds to years [a/s].

The outdoor air concentration for a receptor is expressed the maximum outdoor concentration associated with any field or surface waterbody and is described by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor}}(\mathrm{t}) = \max_{\substack{all\ f \\ all\ sw}} \left(\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,f}}(\mathrm{t}) , \mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,sw}}(\mathrm{t})\right) \tag{5-55}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor}}(t)$	is the outdoor air concentration for lifestyle l [mol/m$^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,f}}(\mathrm{t})$	is the concentration of contaminant j in the air above field f for lifestyle l [mol/ m$^3_{\mathrm{air}}$] described by Equation (5-48); and
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,outdoor,sw}}(\mathrm{t})$	is the concentration of contaminant j in the air above surface water feature sw for lifestyle l [mol/ m$^3_{\mathrm{air}}$] described by Equation (5-52).

5.2.11.2 Indoor Air Concentration

Depending on the lifestyle, indoor air concentration and subsequent exposure to indoor air can be important due to limited air exchange between indoor and outdoor air. The ISM-BIO model assumes indoor air is contaminated via volatile contaminants entering the air via showering and smudging. The total indoor air concentration is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor}}(\mathrm{t}) = \mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,shower}}(t) + \mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,smudge}}(t) \tag{5-56}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor}}(\mathrm{t})$	is the total indoor air concentration for lifestyle l [mol/ m$^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,shower}}(t)$	is the indoor air concentration due to showering for lifestyle l [mol/m$^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,smudge}}(t)$	is the indoor air concentration due to smudging for lifestyle l [mol/m$^3_{\mathrm{air}}$].

5.2.11.2.1 Indoor Air Concentration due to Showering

Showering is a common method of bathing and if a contaminated water source is used for showering contaminants in the water can end up in the shower air via volatilization and aerosolization. The total indoor air concentration in the house is proportional to the frequency of showering and the air exchange rate between the shower and the rest of the house. The indoor air concentration due to showering is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,shower}}(\mathrm{t}) = \frac{N^{l}_{ppl} \cdot sf \cdot t_{shower} \cdot Q_s \cdot C^{j}_{air,shower,vol}(t)}{Q_h} \tag{5-57}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,shower}}(t)$	is the indoor air concentration of contaminant j due to showering [mol/m$^3_{\mathrm{air}}$];
N^{l}_{ppl}	is the number of people in the lifestyle group [-];
sf	is the daily household shower frequency per person [day^{-1}]
t_{shower}	is the shower length [min$_{\mathrm{shower}}$];
Q_s	is the shower air loss rate [m$^3_{\mathrm{air}}$/min$_{\mathrm{shower}}$];
$C^{j}_{air,shower,vol}$	is the shower air concentration of contaminant j due to volatilization for lifestyle l [mol/m$^3_{\mathrm{air}}$] given by Equation (5-58); and
Q_h	is the residence air loss rate [m$^3_{\mathrm{air}}$/day].

The shower air concentration is due volatilization and aerosolization of contaminants in the shower water and is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower}}(\mathrm{t}) = \mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,vol}}(t) + \mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,aero}}(t) \tag{5-58}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower}}(t)$	is the shower air concentration of contaminant j and lifestyle l [mol/ $\mathrm{m}^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,vol}}(t)$	is the shower air concentration of contaminant j due to volatilization for lifestyle l [mol/ $\mathrm{m}^3_{\mathrm{air}}$] given by Equation (5-59); and
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,aero}}(t)$	is the shower air concentration of contaminant j due to aerosolization for lifestyle l [mol/$\mathrm{m}^3_{\mathrm{air}}$] given by Equation (5-60).

The shower air concentration due to volatilization is given by (based on Equation 2-30 from EPA 2000):

$$\mathrm{C}^{\mathrm{j}}_{\mathrm{air,shower,vol}}(t) = \frac{\mathrm{C}^{\mathrm{j,l}}_{\mathrm{dom}}(t)}{\dfrac{1}{H_c^j \rho_{\mathrm{wat}}} + \dfrac{Q_s}{Q_w\left(1 - e^{-\frac{K_l A^j}{Qw}}\right)}} \tag{5-59}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,vol}}(t)$	is the shower air concentration of contaminant j due to volatilization for lifestyle l [mol/ $\mathrm{m}^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{dom}}(t)$	is the domestic use water concentration of contaminant j and lifestyle l [mol/$\mathrm{kg}_{\mathrm{water}}$] given by Equation (5-18);
H_c^j	is the Henry's law constant for contaminant j [$\mathrm{m}^3_{\mathrm{water}}$/$\mathrm{m}^3_{\mathrm{air}}$];
ρ_{wat}	is the density of water [$\mathrm{kg}_{\mathrm{water}}$/$\mathrm{m}^3_{\mathrm{water}}$];
Q_s	is the shower air loss rate [$\mathrm{m}^3_{\mathrm{air}}$/$\mathrm{min}_{\mathrm{shower}}$];
Q_w	is the shower water flow rate [$\mathrm{kg}_{\mathrm{water}}$/$\mathrm{min}_{\mathrm{shower}}$]; and
$K_l A^j$	is the overall mass transfer coefficient for contaminant j [kg/$\mathrm{min}_{\mathrm{shower}}$].

The shower air concentration due to aerosolization is given by (based on Equation 2 of Davis et al. 2016):

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,aero}}(t) = \frac{\lambda_{Aerosol}}{AR \cdot V_{shower}}\,\mathrm{C}^{\mathrm{j,l}}_{\mathrm{dom}}(t) \tag{5-60}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,shower,aero}}(t)$	is the shower air concentration of contaminant j due to aerosolization for lifestyle l [mol/ $\mathrm{m}^3_{\mathrm{air}}$];
$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{dom}}(t)$	is the domestic use water concentration of contaminant j and lifestyle l [mol/$\mathrm{kg}_{\mathrm{water}}$] given by Equation (5-18);
$\lambda_{Aerosol}$	is the aerosol production rate [$\mathrm{kg}_{\mathrm{water}}$/$\mathrm{min}_{\mathrm{shower}}$];
AR	is the aerosol loss rate constant [$\mathrm{min}_{\mathrm{shower}}^{-1}$]; and
V_{shower}	is the shower air volume [$\mathrm{m}^3_{\mathrm{air}}$].

5.2.11.2.2 Indoor Air Concentration due to Smudging

Smudging can be an important practice for some lifestyle and consists of burning small amounts of dried plants such as tobacco, cedar, sweetgrass and sage. This pathway assumes the plants used for smudging are harvested from the garden or forage field and conservatively assumes all contaminants in the plants are volatilized into the air when the smudge is burned. The indoor air concentration due to smudging is given by:

$$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,smudge}}(t) = \frac{N^{l}_{ppl} \cdot \sum_{p} w^{p}_{smudge} \cdot C^{j,l}_{p}(t)}{Q_h} \tag{5-61}$$

where,

$\mathrm{C}^{\mathrm{j,l}}_{\mathrm{air,indoor,smudge}}(t)$	is the indoor air concentration due to smudging for lifestyle l [mol/kg$_{\mathrm{dw}}$];
N^{l}_{ppl}	is the number of people in the lifestyle group [-];
w^{p}_{smudge}	is the amount of plant p used for smudging [kg/day];
$C^{j,l}_{p}(t)$	is the concentration of contaminant j in plant type p for lifestyle l; and
Q_h	is the residence air loss rate [m^3/day].

5.2.12 Concentration in Plants and Animals

The concentration in plants and animals (livestock and wildlife) is calculated based on the concentrations in environmental media estimated using the methodologies described in Sections 5.2.2 to 5.2.11.

5.2.12.1 Concentration in Plants

Plants are assumed to be consumed by humans and animals. For each plant p, the concentration of radionuclide i is given by the following equation:

$$\mathrm{C}^{i,\mathrm{l}}_{\mathrm{p}}(\mathrm{t}) = \mathrm{C}^{i,\mathrm{l}}_{\mathrm{irr}}(t) \cdot \mathrm{P}^{i,\mathrm{p}}_{\mathrm{irr}} + \mathrm{C}^{i,\mathrm{l}}_{\mathrm{soil,f}}(\mathrm{t}) \cdot \mathrm{P}^{i,\mathrm{p}\in\mathrm{f}}_{\mathrm{soil}} + \mathrm{C}^{i,\mathrm{l}}_{\mathrm{air,outdoor,f}}(\mathrm{t}) \cdot \mathrm{P}^{i,\mathrm{p}\in\mathrm{f}}_{\mathrm{air}} \tag{5-62}$$

where,

$\mathrm{C}^{\mathrm{i,l}}_{\mathrm{p}}(t)$	is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg$_{\mathrm{plant\text{-}fw}}$];
$\mathrm{C}^{\mathrm{i,l}}_{\mathrm{irr}}(t)$	is the concentration of radionuclide i in the irrigation water for lifestyle l [Bq/kg$_{\mathrm{water}}$] given by Equation (5-20);
$\mathrm{C}^{\mathrm{i,l}}_{\mathrm{soil,f}}(t)$	is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg$_{\mathrm{soil\text{-}\text{-}dw}}$] given by Equation (5-39);
$\mathrm{C}^{i,\mathrm{l}}_{\mathrm{air,outdoor,f}}(t)$	is the air concentration of radionuclide i in the outdoor air above field f for lifestyle l [Bq/m$^3_{\mathrm{air}}$] given by Equation (5-48);
$\mathrm{P}^{\mathrm{i,p}}_{\mathrm{irr}}$	is the transfer parameter for the irrigation water concentration to the plant concentration for radionuclide j [kg$_{\mathrm{water}}$/kg$_{\mathrm{plant\text{-}fw}}$] given by Equation (5-63);
$\mathrm{P}^{i,\mathrm{p}\in\mathrm{f}}_{\mathrm{soil}}$	is the transfer parameter for soil concentration to plant concentration for the subset of plants grown in field f (p ∈ f) for radionuclide j [kg$_{\mathrm{soil\text{-}dw}}$/kg$_{\mathrm{plant\text{-}fw}}$] given by Equation (5-65); and

$\mathrm{P}_{\mathrm{air}}^{i,\mathrm{p}\in\mathrm{f}}$	is the transfer parameter for air concentration to plant concentration for the subset of plants grown in field f ($\mathrm{p} \in \mathrm{f}$) for radionuclide j [$\mathrm{m}^3_{\mathrm{air}}/\mathrm{kg}_{\mathrm{plant\text{-}fw}}$] given by Equation (5-66).

The transfer from water to plants occurs as a result of irrigation of the plants. It is assumed that the plant retains a volume of water that is proportional to the leaf area, every time plants are irrigated. The transfer parameter for irrigation water to plants ($\mathrm{P}_{\mathrm{irr}}^{\mathrm{i,p}}$) is given by the following equation (Equation 7-13 from Clause 7.3.1.1 of CSA 2020):

$$\mathrm{P}_{\mathrm{irr}}^{j,\mathrm{p}} = \frac{\delta_f \cdot \mathrm{LAI} \cdot \mathrm{I}_{\mathrm{wt}} \cdot \mathrm{\eta}_{\mathrm{I}} \cdot \mathrm{tf} \cdot \mathrm{hi} \cdot \left[1 - \mathrm{e}^{-\lambda_{\mathrm{e}}^{i,\mathrm{p}} \cdot \mathrm{t}_{\mathrm{e}}^{\mathrm{wet}}}\right]}{\lambda_{\mathrm{e}}^{\mathrm{i,p}} \cdot \mathrm{Y}_{\mathrm{p}}} \tag{5-63}$$

where,

$\mathrm{P}_{\mathrm{irr}}^{i,\mathrm{p}}$	is the transfer parameter for the irrigation water concentration to the plant concentration [$\mathrm{kg}_{\mathrm{water}}/\ \mathrm{kg}_{\mathrm{plant\text{-}fw}}$];
δ_f	is a Boolean parameter that is 1 if a farm field is used and zero if instead a wetland is converted to farm field;
LAI	is the leaf area index (leaf area per unit surface area) [$\mathrm{m}^2_{\mathrm{leaf}}/\mathrm{m}^2_{\mathrm{soil}}$];
I_{wt}	is the mass of water retained per unit leaf area [$\mathrm{kg}_{\mathrm{water}}/\mathrm{m}^2_{\mathrm{leaf}}$];
$\mathrm{\eta}_{\mathrm{I}}$	is the frequency of irrigation events per year [1/a];
tf	is the translocation factor from foliage to consumable product [-];
hi	is the harvest index (mass of consumable product divided by mass of total above-ground plant [-];
$\lambda_{\mathrm{e}}^{i,\mathrm{p}}$	is the effective removal constant from vegetation surfaces for radionuclide i and plant p [1/a];
Y_{p}	is the plant yield density for plant p [$\mathrm{kg}_{\mathrm{plant\text{-}fw}}\ /\mathrm{m}^2_{\mathrm{soil}}$]; and
$\mathrm{t}_{\mathrm{e}}^{\mathrm{wet}}$	is the effective duration of the wet deposition [a].

The effective removal constant from vegetation surfaces is the sum of the radioactive decay constant, and the removal constant from vegetation surfaces (considers removal processes such as wind, rain, and plant growth). Thus:

$$\lambda_{\mathrm{e}}^{i,\mathrm{p}} = \lambda_i + \lambda_{\mathrm{veg}}^{\mathrm{p}} \tag{5-64}$$

where,

$\lambda_{\mathrm{e}}^{i,\mathrm{p}}$	is the effective removal constant from vegetation surfaces for radionuclide i and plant p [1/a];
λ_{i}	is the radioactive decay constant for radionuclide i [1/a]; and
$\lambda_{\mathrm{veg}}^{\mathrm{p}}$	is the removal constant from vegetation surfaces for plant p [1/a].

Radionuclides are transferred from the soil to plants through uptake by the roots. The transfer parameter that describes this process ($\mathrm{P}_{\mathrm{soil}}^{\mathrm{i,p}}$) is given by the following equation (Equation 6-62 from Clause 6.8.1 of CSA 2020):

$$\mathrm{P}_{\mathrm{soil}}^{i,\mathrm{p}} = \mathrm{CR}_{\mathrm{p}}^{i} \tag{5-65}$$

where,

$\mathrm{P}_{\mathrm{soil}}^{\mathrm{i,p}}$	is the transfer parameter for soil concentration to plant concentration for radionuclide i [$\mathrm{kg}_{\mathrm{soil\text{-}dw}}/\mathrm{kg}_{\mathrm{plant\text{-}fw}}$]; and
$\mathrm{CR}_{\mathrm{p}}^{i}$	is the plant/soil concentration ratio of radionuclide j for plant p [$\mathrm{kg}_{\mathrm{soil\text{-}dw}}/\mathrm{kg}_{\mathrm{plant\text{-}fw}}$].

Radionuclides are transferred from air to plants through dry deposition. The transfer parameter that describes this process ($\mathrm{P}_{\mathrm{air}}^{\mathrm{i,p}}$) is given by the following equation from Clause 6.4.1 of CSA (2020):

$$\mathrm{P}_{\mathrm{air}}^{i,\mathrm{p}} = \frac{\mathrm{v}_g \cdot \mathrm{f}_{\mathrm{int}} \cdot \mathrm{tf} \cdot \mathrm{hi} \cdot \left[1 - \mathrm{e}^{-\lambda_{\mathrm{e}}^{i,\mathrm{p}} \cdot \mathrm{t}_{\mathrm{e}}^{\mathrm{dry}}}\right]}{\lambda_{\mathrm{e}}^{j,\mathrm{p}} \cdot \mathrm{Y}_{\mathrm{p}}} \tag{5-66}$$

where,

$\mathrm{P}_{\mathrm{air}}^{i,\mathrm{p}}$	is the transfer parameter for air concentration to plant concentration for radionuclide i [$\mathrm{m}^3/\mathrm{kg}_{\mathrm{plant\text{-}fw}}$];
v_g	is the deposition velocity [m/a];
$\mathrm{f}_{\mathrm{int}}$	is the foliar intersection fraction [-];
$\mathrm{t}_{\mathrm{e}}^{\mathrm{dry}}$	is the effective duration of the dry deposition [a]; and
tf, hi, $\lambda_{\mathrm{e}}^{i,\mathrm{p}}$, Y_{p}	are as defined in Equation (5-63).

According to Equation 6-31a from Clause 6.3.3.1 of CSA (2020), the deposition velocity is a combination of the dry deposition velocity and the wet deposition velocity as follows:

$$\mathrm{v}_g = \mathrm{v}_d + \mathrm{v}_w \tag{5-67}$$

where,

v_g	is the deposition velocity [$\mathrm{m}_{\mathrm{soil}}/\mathrm{a}$];
v_d	is the dry deposition velocity [$\mathrm{m}_{\mathrm{soil}}/\mathrm{a}$]; and
v_w	is the wet deposition velocity [$\mathrm{m}_{\mathrm{soil}}/\mathrm{a}$].

The wet deposition velocity is described in terms of the washout ratio and the precipitation rate as follows (based on Equation 6-31b from Clause 6.3.3.1 of CSA (2020)):

$$\mathrm{v}_w = W_r \cdot P_{tot} \tag{5-68}$$

where,

W_r	is the washout ratio [-]; and
P_{tot}	is the annual precipitation rate [$\mathrm{m}_{\mathrm{soil}}/\mathrm{a}$].

5.2.12.2 Concentration in Animals

The biosphere model considers animal tissue concentrations because humans can receive a dose from the ingestion of contaminated animal meat. The biosphere model considers both livestock and wildlife animals which are exposed through slightly different pathways.

5.2.12.2.1 Concentration in Livestock

The concentration of radionuclide j in livestock tissue is given by the following equation:

$$\mathrm{C}_{\mathrm{ls}}^{i,\mathrm{l}}(\mathrm{t}) = \mathrm{C}_{\mathrm{air,outdoor,f}}^{\mathrm{i,l}}(\mathrm{t}) \cdot \mathrm{P}_{\mathrm{air}}^{\mathrm{ls}} + \mathrm{C}_{\mathrm{p}}^{i,\mathrm{l}}(\mathrm{t}) \cdot \mathrm{P}_{\mathrm{p}}^{i,\mathrm{ls}} + \mathrm{C}_{\mathrm{soil,f}}^{i,\mathrm{l}}(\mathrm{t}) \cdot \mathrm{P}_{\mathrm{soil}}^{\mathrm{ls}} + (\mathrm{t}) \cdot \mathrm{P}_{lw}^{\mathrm{ls}} \tag{5-69}$$

where,

$\mathrm{C}_{\mathrm{ls}}^{\mathrm{i,l}}(t)$	is the concentration of radionuclide i in livestock ls for lifestyle l [Bq/kg$_{\text{livestock-fw}}$];
$\mathrm{C}_{\mathrm{air,outdoor,f}}^{i,\mathrm{l}}(t)$	is the air concentration of radionuclide i in the outdoor air above field f for lifestyle l [Bq/m$^3_{\text{air}}$] given by Equation (5-48);
$\mathrm{C}_{\mathrm{p}}^{\mathrm{i,l}}(t)$	is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg$_{\text{plant-fw}}$] given by Equation (5-62);
$\mathrm{C}_{\mathrm{soil,f}}^{\mathrm{i,l}}(t)$	is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg$_{\text{soil--dw}}$] given by Equation (5-39);
$\mathrm{C}_{\mathrm{lw}}^{\mathrm{i,l}}(t)$	is the concentration of radionuclide i in the livestock water for lifestyle l [Bq/kg$_{\text{water}}$] given by Equation (5-19);
$\mathrm{P}_{\mathrm{air}}^{\mathrm{ls}}$	is the transfer parameter for air concentration to livestock ls tissue concentration [kg$_{\text{plant-dw}}$/kg$_{\text{plant-dw}}$] given by Equation (5-70);
$\mathrm{P}_{\mathrm{p}}^{i,\mathrm{ls}}$	is the transfer parameter for plant concentration to livestock ls tissue concentration for radionuclide i [kg$_{\text{plant-dw}}$/kg$_{\text{plant-dw}}$] given by Equation (5-71);
$\mathrm{P}_{\mathrm{soil}}^{\mathrm{ls}}$	is the transfer parameter for soil concentration to livestock ls tissue concentration [kg$_{\text{soil-dw}}$/kg$_{\text{livestock-fw}}$] given by Equation (5-72); and
$\mathrm{P}_{\mathrm{lw}}^{\mathrm{ls}}$	is the transfer parameter for livestock water concentration to livestock ls tissue concentration [kg$_{\text{water}}$/kg$_{\text{livestock-fw}}$] given by Equation (5-73).

Radionuclides are transferred from the air to the livestock tissue through inhalation. The transfer parameter that describes this process is given by the following equation (Equation 6-75 form Clause 6.12.1.1 of CSA 2020):

$$\mathrm{P}_{\mathrm{air}}^{\mathrm{ls}} = \mathrm{R}_{\mathrm{inh}}^{\mathrm{ls}} \cdot \mathrm{F}_{\mathrm{inh}}^{\mathrm{ls}} \tag{5-70}$$

where,

$\mathrm{P}_{\mathrm{air}}^{\mathrm{ls}}$	is the transfer parameter for air concentration to livestock ls tissue concentration for radionuclide j [m$^3_{\text{air}}$/kg$_{\text{livestock-fw}}$];
$\mathrm{R}_{\mathrm{inh}}^{\mathrm{ls}}$	is the livestock inhalation rate [m$^3_{\text{air}}$/a]; and
$\mathrm{F}_{\mathrm{inh}}^{\mathrm{ls}}$	is the fraction of the livestock's annual intake by inhalation that appears in each kg of produce [a/kg$_{\text{livestock-fw}}$].

Radionuclides are also transferred from plants to livestock tissue from consumption of plants. The transfer parameter that describes this process is given by the following equation (Equation 6-68 from Clause 6.10.1.1 of CSA 2020):

$$\mathrm{P}_{\mathrm{p}}^{i,\mathrm{ls}} = \frac{\mathrm{f}_{\mathrm{feed}} \cdot \mathrm{R}_{\mathrm{ing,feed}}^{\mathrm{ls}} \cdot \mathrm{F}_{\mathrm{ing}}^{\mathrm{i,ls}} \cdot \mathrm{e}^{-\lambda_i \cdot \mathrm{t}_h}}{\mathrm{DW}_{\mathrm{p}}} \tag{5-71}$$

where,

$\mathrm{P}_{\mathrm{p}}^{i,\mathrm{ls}}$	is the transfer parameter for plant concentration to livestock ls tissue concentration for radionuclide i [$\mathrm{kg_{plant\text{-}fw}/kg_{plant\text{-}dw}}$];
$\mathrm{f_{feed}}$	is the fraction of feed from contaminated source [-];
$\mathrm{R_{ing,feed}^{ls}}$	is the livestock ls ingestion rate of feed [$\mathrm{kg_{plant\text{-}dw}/a}$];
$\mathrm{F_{ing}^{i,ls}}$	is the fraction of the livestock's annual intake by ingestion that appears in each kg of livestock [$\mathrm{a/kg_{livestock\text{-}fw}}$];
λ_i	is the radioactive decay constant of radionuclide i [1/a];
t_h	is the hold-up time between plant exposure to contamination and feeding [a]; and
$\mathrm{DW_p}$	is the dry/fresh weight ratio for plant p [$\mathrm{kg_{plant\text{-}dw}/kg_{plant\text{-}fw}}$].

Radionuclides are transferred from soil to livestock tissue from the consumption of soil. The transfer parameter that describes this process is given by the following equation (Equation 6-73 from Clause 6.11.1.1 of CSA 2020):

$$\mathrm{P_{soil}^{ls}} = \left(\mathrm{f_{feed}} \cdot \mathrm{R_{ing,feed}^{ls}} \cdot \mathrm{f_{sl}} + \mathrm{R_{ing,soil}^{ls}}\right) \cdot \mathrm{F_{ing}^{ls}} \tag{5-72}$$

where,

$\mathrm{P_{soil}^{ls}}$	is the transfer parameter for soil concentration to livestock ls tissue concentration for radionuclide I [$\mathrm{kg_{soil\text{-}dw}/kg_{livestock\text{-}fw}}$];
$\mathrm{f_{feed}}$	is the fraction of feed from contaminated sources [-];
$\mathrm{R_{ing,feed}^{ls}}$	is the livestock ls ingestion rate of feed [$\mathrm{kg_{feed\text{-}dw}/a}$];
$\mathrm{f_{sl}}$	is the soil load on feed as consumed [$\mathrm{kg_{soil\text{-}dw}/kg_{feed\text{-}dw}}$];
$\mathrm{R_{ing,soil}^{ls}}$	is the livestock ls ingestion rate of soil [$\mathrm{kg_{soil\text{-}dw}/a}$]; and
$\mathrm{F_{ing}^{ls}}$	is the fraction of the livestock's annual intake by ingestion that appears in each kg of livestock [$\mathrm{a/kg_{livestock\text{-}fw}}$].

Radionuclides are transfers from water to livestock from the consumption of water. The transfer parameter that describes this process is given by the following equation (Equation 6-64 from Clause 6.9.1.1 of CSA 2020):

$$\mathrm{P}_{lw}^{\mathrm{ls}} = f_w \cdot \mathrm{R_{ing,wat}^{ls}} \cdot \mathrm{F_{ing}^{ls}} \tag{5-73}$$

where,

$\mathrm{P_{lw}^{ls}}$	is the transfer parameter for livestock water concentration to livestock ls tissue concentration [$\mathrm{kg_{water}/kg_{livestock\text{-}fw}}$];
f_w	is the fraction of water from contaminated sources [-];
$\mathrm{R_{ing,wat}^{ls}}$	is the livestock ls ingestion rate of water [$\mathrm{kg_{water}/a}$]; and
$\mathrm{F_{ing}^{ls}}$	is the fraction of the livestock's annual intake by ingestion that appears in each kg of livestock [$\mathrm{a/kg_{livestock\text{-}fw}}$].

5.2.12.2.2 Aquatic Biota

The aquatic biota considered in the ISM-BIO model are aquatic plants and fish. The fish are consumed by humans and wildlife, and the aquatic plants are consumed by wildlife.

The concentration in aquatic biota is given by the following equation:

$$\mathrm{C^{i}_{ab}(t) = C^{i,l}_{msw}}(t) \cdot \mathrm{P^{i,ab}_{msw}} \tag{5-74}$$

where,

$\mathrm{C^{i}_{ab}}(t)$	is the concentration of radionuclide i in the aquatic biota [Bq/kg$_{\text{ab-fw}}$];
$\mathrm{C^{i,l}_{msw}}(t)$	is the concentration of radionuclide i in the main surface waterbody for lifestyle l [Bq/kg$_{\text{water}}$] given by Equation (5-16); and
$\mathrm{P^{i,ab}_{msw}}$	is the transfer parameter for the main surface waterbody concentration to aquatic biota tissue concentration for radionuclide i [kg$_{\text{water}}$/kg$_{\text{ab-fw}}$] given by Equation (5-75).

The transfer parameter for water to aquatic biota is described by a bioaccumulation factor for each aquatic biota and radionuclide i (Equation 7-20 from Clause 7.7.1 of CSA 2020):

$$\mathrm{P^{i,ab}_{msw} = BAF^{i}_{ab}} \tag{5-75}$$

where,

$\mathrm{BAF^{i}_{ab}}$	is the bioaccumulation factor of radionuclide I in aquatic biota ab [Bq/kg$_{\text{ab-fw}}$].

5.2.12.2.3 Wildlife

The transfer of radionuclides to wildlife is very similar to the transfer of radionuclides to livestock, except that wildlife also eat aquatic biota and drink surface water rather than domestic water. Therefore, the equation that describes the concentration of radionuclides in wildlife is as follows:

$$\mathrm{C^{i,l}_{wl}(t) = C^{i,l}_{air,outdoor,f}(t)P^{wl}_{air}} + \mathrm{C}^{i,\mathrm{l}}_{\mathrm{p}}\mathrm{(t)P}^{i,\mathrm{wl}}_{\mathrm{p}} + \mathrm{C}^{i,\mathrm{l}}_{\mathrm{soil,f}}\mathrm{(t)P}^{wl}_{\mathrm{soil}} + \mathrm{C}^{i,\mathrm{l}}_{\mathrm{ab}}\mathrm{(t)P}^{wl}_{\mathrm{ab}} + \mathrm{C}^{i,\mathrm{l}}_{msw}\mathrm{(t)P}^{wl}_{\mathrm{msw}} \tag{5-76}$$

where,

$\mathrm{C^{i,l}_{wl}}$	is the concentration of radionuclide i in the wildlife wl for lifestyle l [Bq/kg$_{\text{wildlife-fw}}$];
$\mathrm{C}^{i,\mathrm{l}}_{\mathrm{air,outdoor,f}}(t)$	is the air concentration of radionuclide i in the outdoor air above field f for lifestyle l [Bq/m$^{3}_{\text{air}}$] given by Equation (5-48);
$\mathrm{C^{i,l}_{p}}(t)$	is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg$_{\text{plant-fw}}$] given by Equation (5-62);
$\mathrm{C^{i,l}_{soil,f}}(t)$	is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg$_{\text{soil--dw}}$] given by Equation (5-39);
$\mathrm{C^{i}_{ab}}(t)$	is the concentration of radionuclide i in the aquatic biota [mol/kg$_{\text{water}}$] given by Equation (5-74);
$\mathrm{C^{i,l}_{msw}}(t)$	is the concentration of radionuclide i in the main surface waterbody for lifestyle l [mol/kg$_{\text{water}}$] given by Equation (5-16);
$\mathrm{P^{i,wl}_{air}}$	is the transfer parameter for air concentration to wildlife wl tissue concentration for radionuclide i [m^{3}/kg$_{\text{wildlife-fw}}$] given by Equation (5-70);
$\mathrm{P^{i,wl}_{p}}$	is the transfer parameter for plant p concentration to wildlife wl tissue concentration for radionuclide i [-] given by Equation (5-71);
$\mathrm{P^{i,wl}_{ab}}$	is the transfer parameter for aquatic biota to wildlife tissue [-] given by Equation (5-77);

$P_{soil}^{i,wl}$ is the transfer parameter from soil concentration to wildlife tissue concentration for radionuclide i [$kg_{soil\text{-}dw}/kg_{wildlife\text{-}fw}$] given by Equation (5-72); and

$P_{msw}^{i,wl}$ is the transfer parameter for the main surface water concentration to wildlife wl tissue concentration for radionuclide i [$kg_{water}/kg_{wildlife\text{-}fw}$] given by Equation (5-73).

The transfers from air, plant, soil and water are similar as those described in Equations (5-70) to (5-73) respectively, except that the "ls" (livestock) superscript is replaced by "wl" (wildlife) or the "dom" (domestic) subscript is replaced with "msw" (main surface waterbody). The transfer to wildlife from the consumption of aquatic biota ($P_{ab}^{i,wl}$) is described as follows (derived from Equation 6-68 of Clause 6.10.1.1 of CSA 2020):

$$P_{ab}^{wl} = \frac{f_{ab} \cdot R_{ing,ab}^{wl} \cdot F_{ing}^{wl} \cdot f_{ing,ab}^{wl}}{DW_{ab}} \tag{5-77}$$

where,

P_{ab}^{wl} is the transfer parameter for aquatic biota to wildlife tissue [-];

f_{ab} is the fraction of aquatic biota ab from contaminated sources [-];

$R_{ing,ab}^{wl}$ is the wildlife ingestion rate of aquatic biota ab [$kg_{ab\text{-}dw}/a$];

F_{ing}^{wl} is the fraction of the wildlife's annual intake by ingestion that appears in each kg of produce [$a/kg_{ab\text{-}fw}$];

$f_{ing,ab}^{wl}$ is the fraction of each aquatic biota in the wildlife's wl diet [-]; and

DW_{ab} is the dry/fresh weight ratio of aquatic biota ab [$kg_{ab\text{-}dw}/kg_{ab\text{-}fw}$].

5.2.13 Human Dose Pathways

Dose consequences to humans are grouped into two broad categories. Internal dose pathways consider the dose consequences from radionuclides entering the body though processes such as ingestion and inhalation. External dose pathways consider dose consequences of an individual being exposed to a contaminated environment such as swimming or bathing in contaminated water.

Figure 5-5 illustrates the internal dose model pathways. Internal doses to humans are due to drinking contaminated water, eating contaminated foods (plants, livestock, wildlife and aquatic biota), inadvertent ingestion of soils and sediments as well as breathing contaminated air (indoor and outdoor). The equations describing the internal dose pathways are included in the following subsections:

- Ingestion – Section 5.2.13.1
  - Food – Section 5.2.13.1.1
  - Water – Section 5.2.13.1.2
  - Soil – Section 5.2.13.1.3
  - Sediment – Section 5.2.13.1.4
- Inhalation – Section 5.2.13.2

Figure 5-6 illustrates the external dose model pathways. External doses to humans are due to immersion in contaminated air (indoor and outdoor), immersion in contaminated waters (swimming and bathing), exposure to contaminated soils (groundshine) and exposure to contaminated beach sediments (beachshine). The equations describing the external dose pathways are included in the following subsections:

- Air Immersion – Section 5.2.13.3
- Water Immersion – Section 5.2.13.4
- Groundshine – Section 5.2.13.5
- Beachshine – Section 5.2.13.6

The total dose to humans is described in Section 5.2.13.7. All dose rates are indexed over three different age groups (adult, child and infant) and multiple lifestyles.

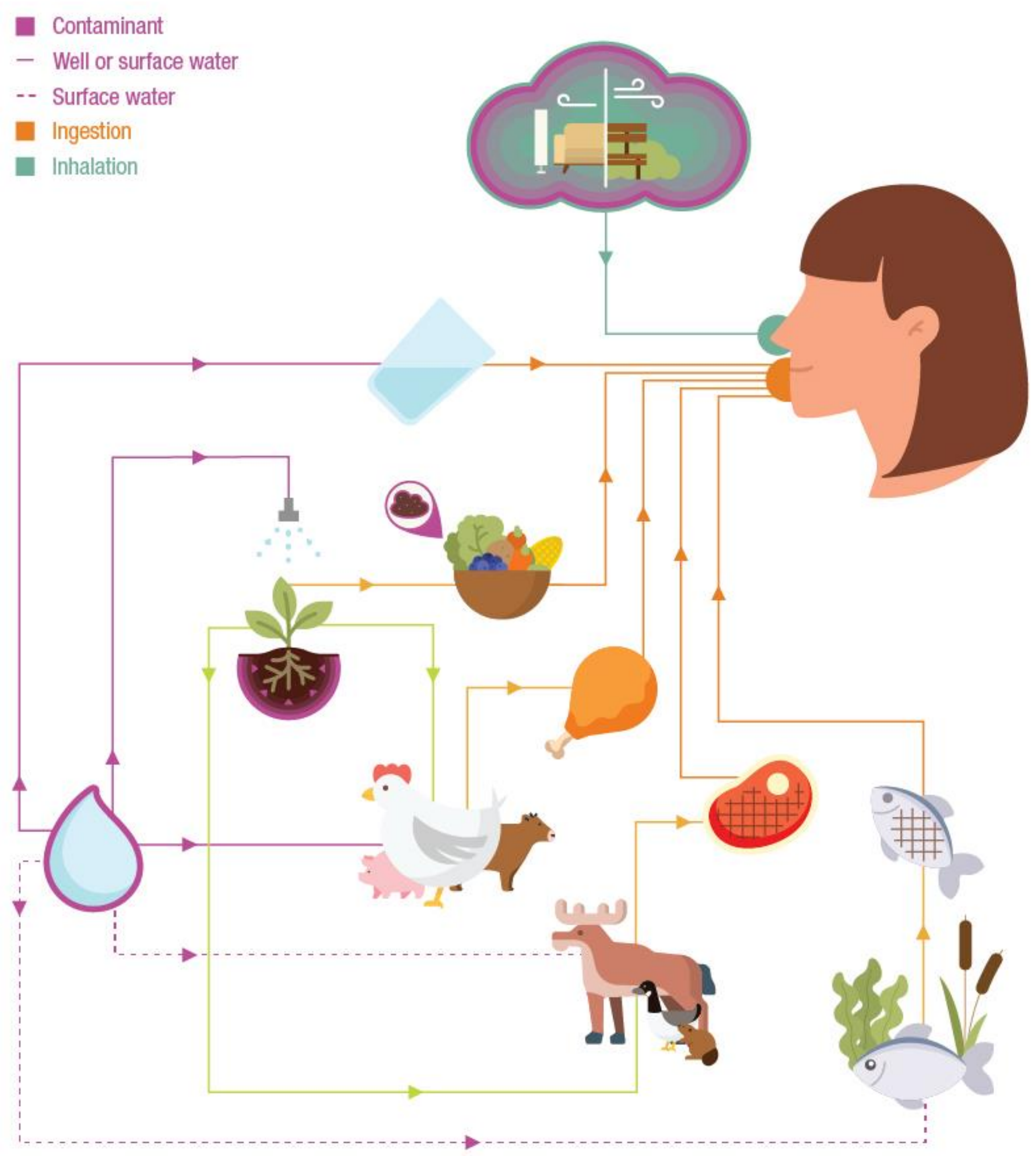

Figure 5-5: Illustration of Internal Dose Model Pathways

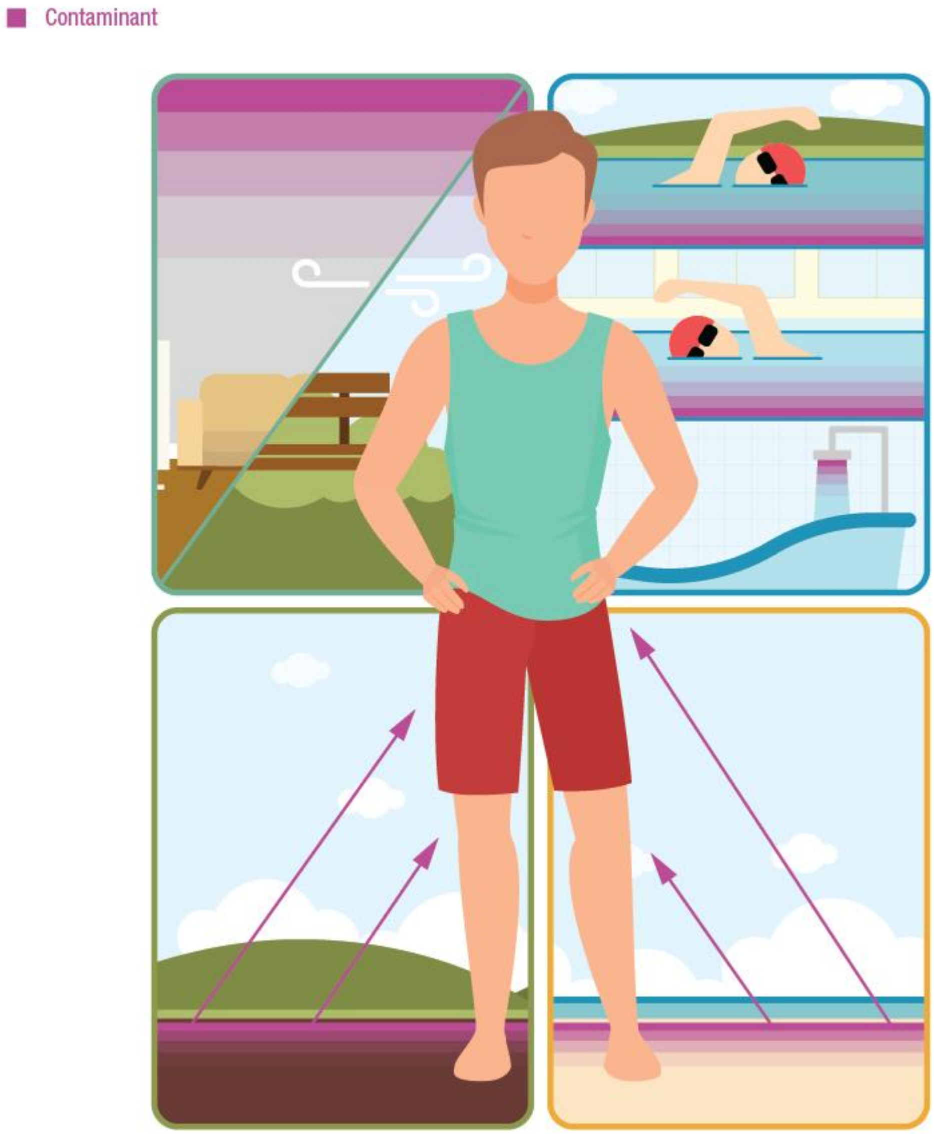

Figure 5-6: Illustration of External Dose Model Pathways

5.2.13.1 Ingestion Dose Rates

Ingestion dose for radionuclide i, lifestyle l, and age group a, arise from the ingestion of food (plants, animals and fish), water, soil and sediment:

$$\begin{aligned}\mathrm{D}_{\mathrm{ing}}^{\mathrm{i,a,l}}(\mathrm{t}) = \sum_{\mathrm{p}} \mathrm{P}_{\mathrm{ing,p}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{p}}^{\mathrm{i,l}}(\mathrm{t}) + \sum_{\mathrm{wl}} \mathrm{P}_{\mathrm{ing,wl}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{wl}}^{\mathrm{i,l}}(\mathrm{t}) + \sum_{\mathrm{ls}} \mathrm{P}_{\mathrm{ing,ls}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{ls}}^{\mathrm{i,l}}(\mathrm{t}) + \sum_{\mathrm{ab}} \mathrm{P}_{\mathrm{ing,ab}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{ab}}^{\mathrm{i}}(\mathrm{t}) \\ + \mathrm{P}_{\mathrm{ing,wat}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{dom}}^{\mathrm{i,l}}(\mathrm{t}) + \mathrm{P}_{\mathrm{ing,soil}}^{\mathrm{i,a,l}} \cdot \max_{all\ f} \mathrm{C}_{\mathrm{soil,f}}^{\mathrm{i,l}}(\mathrm{t}) + \mathrm{P}_{\mathrm{ing,sed}}^{\mathrm{i,a}} \mathrm{C}_{\mathrm{sed}}^{\mathrm{i}}(\mathrm{t})\end{aligned} \tag{5-78}$$

where,

$\mathrm{D}_{\mathrm{ing}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the human dose rate through ingestion for radionuclide i, age group a and lifestyle l [Sv/a];
$\mathrm{C}_{\mathrm{p}}^{\mathrm{i,l}}(\mathrm{t})$	is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg$_{\text{plant-fw}}$] given by Equation (5-62);
$\mathrm{C}_{\mathrm{ls}}^{\mathrm{i,l}}(\mathrm{t})$	is the concentration of radionuclide i in livestock ls for lifestyle l [Bq/kg$_{\text{livestock-fw}}$] given by Equation (5-69);
$\mathrm{C}_{\mathrm{wl}}^{\mathrm{i,l}}(\mathrm{t})$	is the concentration of radionuclide i in wildlife wl for lifestyle l [Bq/kg$_{\text{wildlife-fw}}$] given by Equation (5-76);
$\mathrm{C}_{\mathrm{ab}}^{\mathrm{i}}(\mathrm{t})$	is the concentration of radionuclide i in aquatic biota ab [Bq/kg$_{\text{ab-fw}}$] given by Equation (5-74);
$\mathrm{C}_{\mathrm{dom(t)}}^{\mathrm{i,l}}$	is the concentration of radionuclide i in domestic water for lifestyle l [Bq/kg$_{\text{water}}$] given by Equation (5-18);
$\mathrm{C}_{\mathrm{soil,f}}^{\mathrm{i,l}}(\mathrm{t})$	is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg$_{\text{soil-dw}}$] given by Equation (5-39);
$\mathrm{C}_{\mathrm{sed,beach}}^{\mathrm{i}}(\mathrm{t})$	is the concentration of radionuclide i in beach sediment [Bq/kg$_{\text{sediment-dw}}$] given by Equation (5-21);
$\mathrm{P}_{\mathrm{ing,p}}^{\mathrm{i,a,l}}$	is the transfer parameter for plant concentration to human dose rate through ingestion for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{plant-fw}}$)] given by Equation (5-79);
$\mathrm{P}_{\mathrm{ing,wl}}^{\mathrm{i,a,l}}$	is the transfer parameter for wildlife tissue concentration to human dose rate through ingestion for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{wildlife-fw}}$)] given by Equation (5-79);
$\mathrm{P}_{\mathrm{ing,ls}}^{\mathrm{i,a,l}}$	is the transfer parameter for livestock tissue concentration to human dose rate through ingestion for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{livestock-fw}}$)] given by Equation (5-79);
$\mathrm{P}_{\mathrm{ing,ab}}^{\mathrm{i,a,l}}$	is the transfer parameter from aquatic biota tissue concentration to human dose rate through ingestion of radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{ab-fw}}$)] given by Equation (5-79);
$\mathrm{P}_{\mathrm{ing,wat}}^{\mathrm{i,a,l}}$	is the transfer parameter from water concentration to human dose rate through ingestion of radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{water}}$)] given by Equation (5-80);
$\mathrm{P}_{\mathrm{ing,soil}}^{\mathrm{i,a,l}}$	is transfer parameter from soil concentration to human dose rate through ingestion of radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{soil-dw}}$)] given by Equation (5-81); and

$P^{i,a,l}_{ing,sed}$	is the transfer parameter from sediment to human dose rate through ingestion for radionuclide i age group a, and lifestyle l [(Sv/a)/(Bq/kg$_{\text{sediment-dw}}$)] given by Equation (5-82).

5.2.13.1.1 Food

The transfer parameter for the concentration in food type y to the human dose rate through ingestion for radionuclide i is as follows:

$$P^{i,a,l}_{ing,y} = f_y \cdot f^{y}_{cont} \cdot R^{a,l}_{ing,y} \cdot DCF^{i,a}_{ing} \tag{5-79}$$

where,

$P^{i,a,l}_{ing,y}$	is the transfer parameter for plant concentration to human dose rate through ingestion for radionuclide i, age group a and lifestyle l for food y [(Sv/a)/(Bq/kg$_{\text{food-fw}}$)];
f_y	is the adjustment factor for processing food j [-];
f^{y}_{cont}	is the fraction from contaminated sources of food type j [-];
$R^{a,l}_{ing,y}$	is the ingestion rate of food type j for lifestyle l and age group a [kg$_{\text{food-fw}}$/a];
$DCF^{i,a}_{ing}$	is the dose conversion factor for radionuclide i for intake by ingestion for age group a [Sv/Bq]; and
y	refers to the food type, either plant (p), livestock (ls), wildlife (wl) or aquatic biota (ab).

5.2.13.1.2 Water

The transfer parameter from the water concentration of radionuclide i to human dose rate through ingestion is as follows (Equation 6-81c from Clause 6.15.4.1 of CSA (2020):

$$P^{i,a,l}_{ing,wat} = f_w \cdot R^{a,l}_{ing,wat} \cdot DCF^{i}_{ing} \tag{5-80}$$

where,

$P^{i,a,l}_{ing,wat}$	is the transfer parameter from water concentration to human dose rate through ingestion of radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{water}}$)];
f_w	is the fraction of drinking water from contaminated sources [-];
$R^{a,l}_{ing,wat}$	is the ingestion rate of water for lifestyle l and age group a [kg$_{\text{water}}$/a]; and
$DCF^{i,a}_{ing}$	is the dose conversion factor for radionuclide i for intake by ingestion for age group a [Sv/Bq].

5.2.13.1.3 Soil

The transfer parameter from the soil concentration of radionuclide i to human dose rate through ingestion is as follows (Equation 6-81b from Clause 6.15.4.1 of CSA 2020):

$$P^{i,a,l}_{soil,ing} = R^{a,l}_{ing,soil} \cdot f_{soil} \cdot DCF^{i,a}_{ing} \tag{5-81}$$

where,

$P_{ing,soil}^{i,a,l}$	is transfer parameter from soil concentration to human dose rate through ingestion of radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{soil\text{-}dw}$)];
$R_{ing,soil}^{a,l}$	is the ingestion rate of soil for lifestyle l and age group a [kg$_{soil\text{-}dw}$/a];
f_{soil}	is the fraction of the year where soil ingestion could occur [-]; and
$DCF_{ing}^{i,a}$	is the dose conversion factor for radionuclide i for intake by ingestion for age group a [Sv/Bq].

5.2.13.1.4 Sediment

The transfer parameter from the sediment concentration of radionuclide i to human dose rate through ingestion is as follows (Equation 7-27 from Clause 7.11.1 of CSA 2020):

$$P_{ing,sed}^{i,a,l} = R_{ing,sed}^{a,l} \cdot f_{sed} \cdot DCF_{ing}^{i,a} \tag{5-82}$$

where,

$P_{ing,sed}^{i,a,l}$	is the transfer parameter from sediment to human dose rate through ingestion for radionuclide i age group a, and lifestyle l [(Sv/a)/(Bq/kg$_{sediment\text{-}dw}$)];
$R_{ing,sed}^{a,l}$	is the human ingestion rate of sediment for lifestyle l and age group a [kg$_{sediment\text{-}dw}$/a];
f_{sed}	is the fraction of the year where sediment ingestion could occur [-]; and
$DCF_{ing}^{i,a}$	is the dose conversion factor for radionuclide i for intake by ingestion for age group a [Sv/Bq].

5.2.13.2 Inhalation Dose Rates

Inhalation doses result from the inhalation of outdoor, indoor and shower air. Total inhalation doses are expressed as follows:

$$\begin{aligned} D_{inh}^{i,a,l}(t) = {} & P_{inh,outdoor}^{i,a,l} C_{air,outdoor}^{i,l}(t) \\ & + P_{inh,indoor}^{i,a,l} C_{air,indoor}^{i,l}(t) + P_{inh,shower}^{i,a,l} C_{air,shower}^{i,l}(t) \end{aligned} \tag{5-83}$$

where,

$D_{inh}^{i,a,l}(t)$	is the human dose rate through ingestion for radionuclide i, age group a and lifestyle l [Sv/a];
$C_{air,outdoor}^{i,l}(t)$	is the outdoor air concentration of radionuclide i and lifestyle l [Bq/m$^3_{air}$] given by Equation (5-55);
$C_{air,indoor}^{i,l}(t)$	is the indoor air concentration of radionuclide i and lifestyle l [Bq/m$^3_{air}$] given by Equation (5-56);
$C_{air,shower}^{i,l}(t)$	is the shower air concentration of radionuclide i and lifestyle l [Bq/m$^3_{air}$] given by Equation (5-57);
$P_{inh,outdoor}^{i,a,l}$	is the transfer parameter for outdoor air concentration to dose rate from inhalation for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/m$^3_{air}$)] given by Equation (5-84);
$P_{inh,indoor}^{i,a,l}$	is the transfer parameter for indoor air concentration to dose rate from inhalation for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/m$^3_{air}$)] given by Equation (5-84); and

$P^{i,a,l}_{inh,shower}$ is the transfer parameter for shower air concentration to dose rate from inhalation for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/m^3_{air})] given by Equation (5-84).

The transfer parameter from air to dose rate from inhalation is defined as follows (Equation 6-79 from Clause 6.13.1 of CSA 2020):

$$P^{i,a,l}_{inh,loc} = R^{a}_{inh} \cdot OF_{loc} \cdot DCF^{i,a}_{inh} \tag{5-84}$$

where,

$P^{i,a,l}_{inh,loc}$ is the transfer parameter for a given location's air concentration to dose rate from inhalation for radionuclide i, age group a, and lifestyle l [(Sv/a)/(Bq/m^3_{air})] (note that in this expression location can mean outdoor, indoor or shower);

R^{a}_{inh} is the human's inhalation rate for age group a [m^3_{air}/a];

OF_{loc} is a location's (outdoor, indoor, shower) occupancy factor [-]; and

$DCF^{i,a}_{inh}$ is the dose conversion coefficient for intake by inhalation for radionuclide i for age group a [(Sv)/(Bq)].

5.2.13.3 Air Immersion Rates

The air immersion dose rates are the sum of the outdoor, indoor and shower exposures. It is expressed as follows:

$$\begin{aligned} D^{i,a,l}_{imm,air}(t) = {} & P^{i,a,l}_{imm,outdoor} C^{i,l}_{air,outdoor}(t) \\ & + P^{i,a,l}_{imm,indoor} C^{i,l}_{air,indoor}(t) + P^{i,a,l}_{imm,shower} C^{i,l}_{air,shower}(t) \end{aligned} \tag{5-85}$$

where,

$D^{i,a,l}_{imm,air}(t)$ is the human dose rate through air immersion for radionuclide i, age group a and lifestyle l [Sv/a];

$C^{i,l}_{air,outdoor}(t)$ is the outdoor air concentration of radionuclide i and lifestyle l [Bq/m^3_{air}] given by Equation (5-55);

$C^{i,l}_{air,indoor}(t)$ is the indoor air concentration of radionuclide i and lifestyle l [Bq/m^3_{air}] given by Equation (5-56);

$C^{i,l}_{air,shower}(t)$ is the shower air concentration of radionuclide i and lifestyle l [Bq/m^3_{air}] given by Equation (5-57);

$P^{i,a,l}_{imm,outdoor}$ is the transfer parameter for outdoor air concentration to total rate dose from immersion for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/m^3_{air})] given by Equation (5-86);

$P^{i,a,l}_{imm,indoor}$ is the transfer parameter for indoor air concentration to total rate dose from immersion for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/m^3_{air})] given by Equation (5-86); and

$P^{i,a,l}_{imm,shower}$ is the transfer parameter for shower air concentration to total rate dose from immersion for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/m^3_{air})] given by Equation (5-86);

The transfer parameter from air concentration to the dose rate from immersion in air is calculated as follows (Equation 6-25 from Clause 6.2.1.2 of CSA 2020):

$$P^{i,a,l}_{imm,loc} = OF_{loc} \cdot DCF^{i,a}_{imm,air} \qquad (5\text{-}86)$$

where,

$P^{i,a,l}_{imm}$	is the transfer parameter for a given location's air concentration to dose rate from immersion for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/m$^3_{air}$)] in this expression location can mean outdoor, indoor or shower;
OF_{loc}	is a location's (outdoor, indoor, shower) occupancy factor [-]; and
$DCF^{i,a}_{imm,air}$	is the effective dose conversion coefficient for a semi-infinite cloud for radionuclide i for age group a [(Sv/a)/(Bq/m$^3_{air}$)].

5.2.13.4 Water Immersion Dose Rates

Doses from water immersion results from taking baths and from swimming in surface waters and pools. Baths and swimming pools are assumed to be filled with domestic water, whereas surface waters are assumed to be the main surface waterbody. Therefore, the dose rate from water immersion is expressed as follows:

$$D^{i,a,l}_{Imm,wat}(t) = P^{i,a,l}_{imm,dom} \cdot C^{i,l}_{dom}(t) + P^{i,a,l}_{imm,msw} \cdot C^{i,l}_{msw}(t) \qquad (5\text{-}87)$$

where,

$D^{i,a,l}_{imm,wat}(t)$	is the human dose rate through water immersion for radionuclide i, age group a and lifestyle l [Sv/a];
$C^{i,l}_{dom}(t)$	is the concentration of radionuclide i in domestic water for lifestyle l [Bq/kg$_{water}$] given by Equation (5-18); and
$C^{i,l}_{msw}(t)$	is the concentration of radionuclide i in the main surface waterbody [Bq/kg$_{water}$] given by Equation (5-16).
$P^{i,a,l}_{imm,dom}$	is the transfer parameter for domestic water concentration to water immersion dose rate for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{water}$)] given by Equation (5-88); and
$P^{i,a,l}_{imm,msw}$	is the transfer parameter for the main surface waterbody concentration to water immersion dose rate for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{water}$)] given by Equation (5-89).

The transfer parameter from domestic water concentration to water immersion dose rate is given as follows (Equation 6-82 from Clause 6.16.1.1 of CSA 2020):

$$P^{i,a,l}_{imm,dom} = \left(f_{bath} \cdot OF^{ls}_{bath} + OF^{ls}_{pool}\right) \cdot DCF^{i,a}_{imm,wat} \qquad (5\text{-}88)$$

where,

$P^{i,a,l}_{imm,dom}$	is the transfer parameter for domestic water concentration to water immersion dose rate for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{water}$)];
f_{bath}	is the correction factor to account for the finite size of the bath [-];
OF^{l}_{bath}	is the bath occupancy factor for lifestyle l [-];
OF^{l}_{pool}	is the pool occupancy factor for lifestyle l [-]; and
$DCF^{i,a}_{imm,wat}$	is the dose conversion coefficient for water immersion for radionuclide i [(Sv/a)/(Bq/kg$_{water}$)].

The transfer parameter from the main surface waterbody concentration to the water immersion dose rate is given as follows:

$$\mathrm{P}_{\mathrm{imm,msw}}^{\mathrm{i,a,l}} = \mathrm{OF}_{\mathrm{sw}}^{\mathrm{l}} \cdot \mathrm{DCF}_{\mathrm{imm,wat}}^{\mathrm{i,a}} \tag{5-89}$$

where,

$\mathrm{P}_{\mathrm{imm,msw}}^{\mathrm{i,a,l}}$	is the transfer parameter for the main surface water concentration to water immersion dose rate for radionuclide i, age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\mathrm{water}}$)];
$\mathrm{OF}_{\mathrm{sw}}^{\mathrm{l}}$	is surface water occupancy factor for lifestyle l [-]; and
$\mathrm{DCF}_{\mathrm{imm,wat}}^{\mathrm{i,a}}$	is the dose conversion coefficient for water immersion for radionuclide i [(Sv/a)/(Bq/kg$_{\mathrm{water}}$)].

5.2.13.5 Groundshine Dose Rates

The dose rate due to groundshine is expressed as follows:

$$\mathrm{D}_{\mathrm{gshine}}^{\mathrm{i,a,l}}(\mathrm{t}) = \max_{\mathrm{all\ f}}\left(\mathrm{P}_{\mathrm{gshine,f}}^{\mathrm{i,a,l}} \cdot \mathrm{C}_{\mathrm{soil,f}}^{\mathrm{i,l}}(\mathrm{t})\right) \tag{5-90}$$

where,

$\mathrm{D}_{\mathrm{gshine}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the groundshine human dose rate for radionuclide i, age group a, and lifestyle l [Sv/a];
$\mathrm{C}_{\mathrm{soil,f}}^{\mathrm{i,l}}(\mathrm{t})$	is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg$_{\mathrm{soil\text{-}dw}}$] given by Equation (5-39); and
$\mathrm{P}_{\mathrm{gshine,f}}^{\mathrm{i,a,l}}$	is the transfer parameter for soil concentration of field f to groundshine dose rate for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\mathrm{soil\text{-}dw}}$)] given by Equation (5-91).

The transfer parameter from soil concentration to groundshine dose rate [(Sv/a)/(Bq/kg] is defined as follows (Equation 6-80 from Clause 6.14.1 of CSA (2020):

$$\mathrm{P}_{\mathrm{gshine,f}}^{\mathrm{i,a,l}} = \mathrm{OF}^{l} \cdot \mathrm{f}_{\mathrm{r}} \cdot [\mathrm{OF}_{\mathrm{out}}^{\mathrm{l}} + (1 - \mathrm{OF}_{\mathrm{out}}^{\mathrm{l}}) \cdot \mathrm{S}_{\mathrm{g}}] \cdot \mathrm{Z}_{\mathrm{s}} \cdot \rho_{\mathrm{soil}} \cdot \mathrm{DCF}_{\mathrm{g}}^{\mathrm{i,a}} \tag{5-91}$$

where,

$\mathrm{P}_{\mathrm{gshine,f}}^{\mathrm{i,a,l}}$	is the transfer parameter for soil concentration of field f to groundshine dose rate for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\mathrm{soil\text{-}dw}}$)];
OF^{l}	is the area occupancy factor for lifestyle l [-];
f_{r}	is the dose reduction factor to account for non-uniformity of the grounds surface [-];
$\mathrm{OF}_{\mathrm{out}}^{\mathrm{l}}$	is the outdoor occupancy factor for lifestyle l [-];
S_{g}	is the shielding factor for groundshine, or fraction of the outdoor groundshine received indoors due to shielding by buildings [-];
Z_{s}	is the depth of the surface soil layer [m];
ρ_{soil}	is the soil density [kg$_{\mathrm{dw}}$/m^3]; and
$\mathrm{DCF}_{\mathrm{g}}^{\mathrm{i,a}}$	is the dose conversion coefficient for an infinite plane ground deposit for radionuclide i and age group a [(Sv/a)/(Bq/m^2)].

5.2.13.6 Beachshine Dose Rates

The dose rate due to beachshine, or exposure from sediment while spending time at the beach, is expressed as follows:

$$D_{\mathrm{bshine}}^{\mathrm{i,a,l}}(\mathrm{t}) = P_{\mathrm{bshine}}^{\mathrm{i,a,l}} \cdot C_{\mathrm{sed,beach}}^{\mathrm{i}}(\mathrm{t}) \tag{5-92}$$

where,

$D_{\mathrm{bshine}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the beachshine human dose rate for radionuclide i, age group a, and lifestyle l [Sv/a];
$C_{\mathrm{sed,beach}}^{\mathrm{i}}(\mathrm{t})$	is the concentration of radionuclide i in beach sediment [Bq/kg$_{\text{sediment-dw}}$] given by Equation (5-21); and
$P_{\mathrm{bshine}}^{\mathrm{i,a,l}}$	is the transfer parameter for sediment concentration to beachshine dose rate for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{sediment-dw}}$)] given by Equation (5-93).

The transfer parameter from sediment concentration to beachshine is given by Equation 7-26 from Clause 7.10.1 of CSA (2020) and is defined as follows:

$$P_{\mathrm{bshine}}^{\mathrm{i,a,l}} = OF_{\mathrm{shore}}^{\mathrm{l}} \cdot W_{S} \cdot f_{\mathrm{d}} \cdot DCF_{\mathrm{sed}}^{\mathrm{i,a}} \tag{5-93}$$

where,

$P_{\mathrm{bshine}}^{\mathrm{i,a,l}}$	is the transfer parameter for sediment concentration to beachshine dose rate for radionuclide i for age group a and lifestyle l [(Sv/a)/(Bq/kg$_{\text{sediment-dw}}$)];
$OF_{\mathrm{shore}}^{\mathrm{l}}$	is the shoreline occupancy factor for lifestyle l [-];
W_{S}	is the shore-width factor that describes the shoreline exposure geometry [-];
f_{d}	is the dilution factor for shoreline deposits, which allows for non-equilibrium between suspended sediment and shoreline deposits [-]; and
$DCF_{\mathrm{sed}}^{\mathrm{i,a}}$	is the dose conversion coefficient for uniformly contaminated sediment for radionuclide I and age group a [(Sv/a)/(Bq/kg$_{\text{sediment-dw}}$)].

5.2.13.7 Total Dose Rate

The total dose rates for each age group and lifestyle is given by the sum each radionuclide and dose pathway and is given by:

$$D_{\mathrm{tot}}^{\mathrm{a,l}}(\mathrm{t}) = \sum_{\mathrm{i}} D_{\mathrm{ing}}^{\mathrm{i,a,l}}(\mathrm{t}) + D_{\mathrm{inh}}^{\mathrm{i,a,l}}(\mathrm{t}) + D_{\mathrm{imm,air}}^{\mathrm{i,a,l}}(\mathrm{t}) + D_{\mathrm{imm,wat}}^{\mathrm{i,a,l}}(\mathrm{t}) + D_{\mathrm{gshine}}^{\mathrm{i,a,l}}(\mathrm{t}) + D_{\mathrm{bshine}}^{\mathrm{i,a,l}}(\mathrm{t}) \tag{5-94}$$

where,

$D_{\mathrm{ing}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the human dose rate through ingestion for radionuclide i, age group a and lifestyle l [Sv/a] given by Equation (5-78);
$D_{\mathrm{inh}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the human dose rate through ingestion for radionuclide i, age group a and lifestyle l [Sv/a] given by Equation (5-83);
$D_{\mathrm{imm,air}}^{\mathrm{i,a,l}}(\mathrm{t})$	is the human dose rate through air immersion for radionuclide i, age group a and lifestyle l [Sv/a] given by Equation (5-85);

$\mathrm{D_{imm,wat}^{i,a,l}(t)}$	is the human dose rate through water immersion for radionuclide i, age group a and lifestyle l [Sv/a] given by Equation (5-87);
$\mathrm{D_{gshine}^{i,a,l}(t)}$	is the groundshine human dose rate for radionuclide i, age group a, and lifestyle l [Sv/a] given by Equation (5-90); and
$\mathrm{D_{bshine}^{i,a,l}(t)}$	is the beachshine human dose rate for radionuclide i, age group a, and lifestyle l [Sv/a] given by Equation (5-92).

5.2.14 Specific Activity Models

Exposure to select radionuclides can be limited by environmental or biological processes and reduce the dose one could expect to receive relative to the total dose described in Section 5.2.13.7. Currently the ISM-BIO model includes specific activity models for I-129 and C-14 as described below.

5.2.14.1 I-129 Specific Activity Dose Model

Iodine entering the human body accumulates almost exclusively in the thyroid gland. The internal dose to humans from I-129 can therefore be calculated by considering the thyroid alone (ICRP 1979). Iodine is an essential element and is metabolically regulated so that its concentration in the thyroid stays within narrow limits regardless of intake. Once the thyroid becomes saturated, excess iodine is rapidly excreted from the body.

Stable iodine is present in the environment both in the biosphere and the geosphere. A person’s intake of iodine would therefore involve both active and stable forms. The two forms are handled identically by the body and therefore the thyroid cannot become saturated with I-129 (ICRP, 1979). This can be considered in the iodine dosimetry model for man by implementing a limited specific-activity model in which the ratio of active to stable iodine in the thyroid is set equal to the ratio at intake to the body (Zach and Sheppard 1992). The intake of stable iodine is conservatively set to a low value to increase the specific activity of I-129 and to increase the dose.

In the ISM-BIO model, the I-129 specific activity ingestion dose is described by:

$$\mathrm{D_{ing,sa}^{I129,a,l}(t)} = D_{ing}^{I129,a,l}(t) \cdot \frac{\mathrm{C_{thyroid}^{I}}}{R_{ing}^{I}} \cdot \frac{\mathrm{DCF_{thyroid}^{I129}}}{\mathrm{DCF_{ing}^{I129,a}}} \tag{5-95}$$

where,

$\mathrm{D_{ing,sa}^{I129,a,l}(t)}$	is the I-129 specific activity ingestion dose [Sv/a];
$\mathrm{D_{ing}^{I129,a,l}(t)}$	is the human dose rate through ingestion for I-129, age group a and lifestyle l [Sv/a] given by Equation (5-78);
$\mathrm{C_{thyroid}^{I}}$	is the thyroid iodine concentration [$\mathrm{kg_{iodine}/kg_{thyroid}}$];
$\mathrm{R_{ing}^{I129}}$	is the stable iodine ingestion rate [$\mathrm{kg_{iodine}}$/a];
$\mathrm{DCF_{thyroid}^{I129}}$	is the dose conversion factor for internal dose due to I-129 in the thyroid [(Sv/a)/(Bq/$\mathrm{kg_{thyroid}}$)]; and
$\mathrm{DCF_{ing}^{I129,a}}$	is the dose conversion factor for I-129 for intake by ingestion for age group a [Sv/Bq].

The ISM-BIO model reports the more limiting of the specific activity ingestion dose and the non-specific activity ingestion dose approaches. Specifically:

$$\mathrm{D}_{\mathrm{ing,rep}}^{\mathrm{I129,a,l}}(\mathrm{t}) = \min\left(D_{ing}^{I129,a,l}(t)\,, \mathrm{D}_{\mathrm{ing,sa}}^{\mathrm{I129,a,l}}(\mathrm{t})\right) \tag{5-96}$$

where,

$\mathrm{D}_{\mathrm{ing,rep}}^{\mathrm{I129,a,l}}(\mathrm{t})$	is the reported I-129 ingestion dose from the biosphere model [Sv/a];
$\mathrm{D}_{\mathrm{ing,sa}}^{\mathrm{I129,a,l}}(\mathrm{t})$	is the I-129 specific activity ingestion dose [Sv/a] given by Equation (5-95); and
$\mathrm{D}_{\mathrm{ing}}^{\mathrm{I129,a,l}}(\mathrm{t})$	is the human dose rate through ingestion for I-129, age group a and lifestyle l [Sv/a] given by Equation (5-78).

5.2.14.2 C-14 Specific Activity Dose Model

The C-14 specific activity model implemented in the ISM-BIO model considers the relative amount of C-14 to C-12 throughout the environmental media in the biosphere. The approach used is a hybrid between the C-14 activity model described in CSA N288.1:20 (CSA 2020) and that used by SKB in their safety assessment for the disposal of used nuclear fuel and that for short-lived low and intermediate wastes (SKB 2008).

A hybrid of the two models is needed because the CSA model is intended for nuclear reactor releases and calculates the receiving environmental media specific activities based on point source releases such as a liquid effluent and air plume via a stack release. The SKB models proposes conceptual models appropriate for the diffuse discharges to surface associates with release from a repository. However, SKB (2008) does not have the same detail as the CSA model for transfers within the environment from the receiving environmental media. Consequently, the SKB modeling approach is applied to calculate the field air and surface water concentrations and the CSA model is used to calculate all other environmental concentrations.

The C-14 specific activity model calculates the C-14/C-12 ratio for the environmental media (e.g., well water, surface waters, domestic water, outdoor air above the forage field and garden, and indoor air). For the majority of environmental media, the transfer of C-14 between biosphere compartments and components is not impacted by the C-14 specific activity model. For example, the ratio of C-14 in the well water is given by:

$$r_{well}^{C14/C12}(t) = \frac{C_{well}^{C14,l}(t) \cdot f_{mol-Bq}^{C14}}{C_{well}^{C12}} \tag{5-97}$$

where,

$r_{well}^{C14/C12}(t)$	is the ratio of C-14 to C-12 in a given well (residential or community) [Bq/kg$_{\mathrm{C12}}$];
$C_{well}^{C14,l}(t)$	is concentration of C-14 in a given well (residential or community) water [mol/kg$_{\mathrm{water}}$] given by Equation (5-1) or Equation (5-7);
f_{mol-Bq}^{C14}	is a conversion factor from moles to Bq for C-14 [Bq/mol]; and
C_{well}^{C12}	is the concentration of C-12 in given well water (residential or community) [kg$_{\mathrm{C12}}$/kg$_{\mathrm{water}}$].

The concentration of C-14 in the well water is calculated as:

$$C_{well,sa}^{C14}(t) = r_{well}^{C14/C12}(t) C_{well}^{C12} \tag{5-98}$$

where,

$C_{well,sa}^{C14}(t)$	is the C-14 specific activity concentration in a given well (residential or community) [Bq/kg$_{C12}$].

Equation (5-98) is then equal to Equation (5-1) for the residential well and (5-7) for the community well. Rather than reproduce the entire biosphere model theory for the C-14 described in this report, specific activity model key differences between the general biosphere theory and the C-14 specific activity model are described below.

5.2.14.2.1 C-14 Specific Activity Surface Water Transfers

The C-14 concentration in surface waters is calculated following the same dynamic transfers described in Section 5.2.2 with one notable change, that is the addition of a loss due to primary production (see Figure 5-12). The loss of C-14 due to primary production is given by:

$$\lambda_{NPP,sw}^{C14}(\mathrm{t}) = \frac{NPP_{wat}^{C12}}{C_{sw}^{C12} \cdot \rho_{wat} \cdot Z_{sw}} \tag{5-99}$$

where,

$\lambda_{NPP,sw}^{C14}(\mathrm{t})$	is the loss rate of C-14 from surface water feature sw due to primary production of C-12 [1/a];
NPP_{wat}^{C12}	is the net primary production rate of C-12 in surface waterbodies [kg$_{C12}$/m$^2_{water}$/a];
C_{sw}^{C12}	is the concentration of C-12 in the surface water [kg$_{C12}$/kg$_{water}$];
ρ_{wat}	is the density of water [kg$_{water}$/m$^3_{water}$]; and
Z_{sw}	is the depth of the surface water feature sw [m$_{water}$].

5.2.14.2.2 C-14 Specific Activity Soil Model

Soil is not included as an environmental in the C-14 specific activity model. Instead, all C-14 that would enter the soil is assumed to be redirected to the outdoor air (See Figure 5-12). This is conservative since is maximizes the amount of C-14 that is incorporated into plant tissue through photosynthesis.

5.2.14.2.3 C-14 Specific Activity Outdoor Air Concentration

The C-14 specific activity concentration in the outdoor air is given by:

$$C_{air,outdoor,sa}^{C14,l}(\mathrm{t}) = r_{air,f}^{C14/C12}(t) \cdot C_{air}^{C12} \tag{5-100}$$

where,

$C_{air,outdoor,sa}^{C14,l}(\mathrm{t})$	is the C-14 specific activity concentration in the outdoor air for lifestyle l [Bq/kg] and is equivalent to the outdoor air concentration for other radionuclides given by Equation (5-55);
$r_{air,f}^{C14/C12}(t)$	is the C-14/C-12 ratio in the outdoor air above field f [Bq/kg$_{C12}$] given by Equation (5-101); and

C_{air}^{C12}	is the C-12 concentration in the air [kg_{C12}/m^3_{air}].

The field air C-14 to C-12 ratio is calculated using the equilibrium equation from Section 3.2 of SKB (2008) and depends on the flux from the geosphere, the flux from irrigation, air mixing and the net primary productivity. The equilibrium equation combines Equation 3.1 and 3.6 from SKB (2008) and is defined as:

$$r_{air,f}^{C14/C12}(t) = \frac{\dfrac{\mathrm{X}_{\mathrm{soil,f}}^{C14}(\mathrm{t}) \cdot f_{mol-Bq}^{C14}}{A_f^l} + C_{irr}^{C14,l}(\mathrm{t}) \cdot f_{mol-Bq}^{C14} \cdot R_{irr,f}^{l} \cdot \rho_{wat}}{h \times \left(\dfrac{v \, {}^{\ln\left(h_{veg}/Z_0\right)}\big/_{\ln\left(10/Z_0\right)}}{\sqrt{A_f^l/\pi}} \right) \cdot C_{air}^{C12} + NPP_f^{C12}} \tag{5-101}$$

where,

$r_{air}^{C14/C12,f}(t)$	is the C-14/C-12 ratio in the outdoor air above field f [Bq/kg_{C12}];
$\mathrm{X}_{\mathrm{soil,f}}^{C14}(\mathrm{t})$	is the C-14 discharge rate to the field f [mol/a] given by Equation (5-25);
f_{mol-Bq}^{C14}	is a conversion factor from moles to Bq for C-14 [Bq/mol];
A_f^l	is the area of field f for lifestyle l [m^2_{soil}] given by Equation (5-26) for the garden field and Equation (5-27) for the forage field;
$C_{irr}^{C14,l}(t)$	is the irrigation water concentration [mol/kg_{water}] given by Equation (5-20);
$\mathrm{R}_{\mathrm{irr,f}}^{\mathrm{l}}$	is the irrigation rate of field f for lifestyle l [$m^3_{water}/a/m^2_{soil}$];
ρ_{wat}	is the density of water [kg_{water}/m^3_{water}];
h	is the air mixing height [m_{air}];
v	is the average wind speed at 10 meters height [m/a];
h_{veg}	is the vegetation height [m];
Z_0	is the roughness length [m];
C_{air}^{C12}	is the concentration of C-12 in the air [kg_{C12}/m^3_{air}]; and
NPP_f^{C12}	is the net primary production rate of C-12 in field f [$kg_{C12}/m^2_{soil}/a$].

5.2.14.2.4 C-14 Specific Activity Plant Concentration

The C-14 specific activity plant concentration is given by:

$$C_{p,sa}^{C14,l}(\mathrm{t}) = r_{air,f}^{C14/C12}(t) \cdot C_p^{C12} \tag{5-102}$$

where,

$C_{p,sa}^{C14,l}(\mathrm{t})$	is the C-14 specific activity concentration in plant type p and lifestyle l [$Bq/kg_{plant-fw}$]; is equivalent to plant concentration for other radionuclides given by Equation (5-62);
$r_{air,f}^{C14/C12}(t)$	is the C-14/C-12 ratio in the outdoor air above field f [Bq/kg_{C12}] given by Equation (5-101); and
C_p^{C12}	is the C-12 concentration in plant type p [$kg_{C12}/kg_{plant-fw}$].

5.2.14.2.5 C-14 Specific Activity Aquatic Biota Concentration

The C-14 specific activity aquatic biota concentration is given by:

$$C_{ab,sa}^{C14}(\mathrm{t}) = r_{msw}^{C14/C12,l}(t) \cdot C_{ab}^{C12} \qquad \text{(5-103)}$$

where,

$C_{p,sa}^{C14,l}(\mathrm{t})$	is the C-14 specific activity concentration in aquatic biota type ab [Bq/kg$_{\text{ab-fw}}$] and is equivalent to the aquatic biota concentration for other radionuclides given by Equation (5-74);
$r_{msw}^{C14/C12,l}(t)$	is the C-14/C-12 ratio in the main surface waterbody for lifestyle l [Bq/kg$_{\text{C12}}$] given by Equation (5-104); and
C_{ab}^{C12}	is the C-12 concentration in aquatic biota type ab [kg$_{\text{C12}}$/kg$_{\text{ab-fw}}$].

The C-14 to C-12 ratio in the main surface waterbody is given by:

$$r_{msw}^{C14/C12,l}(t) = \frac{\mathrm{C}_{\mathrm{msw}}^{\mathrm{j}}(t) \cdot f_{mol-Bq}^{C14}}{C_{msw}^{C12}} \qquad \text{(5-104)}$$

where,

$r_{msw}^{C14/C12,l}(t)$	is the ratio of C-14 to C-12 in the main surface waterbody [Bq/kg$_{\text{C12}}$];
$C_{msw}^{C14}(t)$	is concentration of C-14 in the main surface water feature [mol/kg$_{\text{water}}$] given by Equation (5-15);
f_{mol-Bq}^{C14}	is a conversion factor from moles to Bq for C-14 [Bq/mol]; and
C_{msw}^{C12}	is the concentration of C-12 in the surface water [kg$_{\text{C12}}$/kg$_{\text{water}}$].

5.2.14.2.6 C-14 Specific Activity Livestock Concentration

The C-14 specific activity livestock concentration in the biosphere model includes C-14 from ingestion of plants as well as drinking water. Ingestion of sediments and soil as well as inhalation are excluded as they are not a significant source of C-14 (Section 6.11.2 and 6.12.3 of CSA (2020) respectively). CSA (2020) also excludes drinking water a significant source of C-14 for livestock (CSA, Section 7.7.5); however, this pathway is included in the ISM-BIO model for conservatism. The C-14 specific activity livestock concentration due to ingestion feed plants and water is given by:

$$C_{ls,sa}^{C14,l}(\mathrm{t}) = \left(\mathrm{P}_{\mathrm{p,sa}}^{\mathrm{C14,ls}} \cdot \mathrm{C}_{\mathrm{p,sa}}^{\mathrm{C14,l}}(\mathrm{t}) + \mathrm{P}_{\mathrm{dom,sa}}^{\mathrm{ls}} \cdot r_{lw}^{C14/C12,l}(t) \cdot C_{lw}^{C12}\right) \cdot \frac{C_{ls}^{C12}}{R_{ing}^{C12}} \qquad \text{(5-105)}$$

where,

$C_{ls,sa}^{C14,l}(\mathrm{t})$	is the C-14 specific activity in livestock type ls and lifestyle l [Bq/kg$_{\text{livestock-fw}}$] and is equivalent to the livestock concentration for other radionuclides given by Equation (5-69);
$\mathrm{P}_{\mathrm{p,sa}}^{\mathrm{C14,ls}}$	is the C-14 specific activity transfer parameter for plant concentration to livestock tissue concentration for livestock type ls and plant p [kg$_{\text{plant-fw}}$/a] and is given by Equation (5-106);

$\mathrm{C}^{\mathrm{C14,l}}_{\mathrm{p,sa}}(\mathrm{t})$	is the C-14 specific activity concentration in plant p in lifestyle l [Bq/$\mathrm{kg}_{\text{plant-fw}}$] given by Equation (5-102);
$\mathrm{P}^{\mathrm{ls}}_{\mathrm{dom,sa}}$	is the C-14 specific activity transfer parameter for domestic water concentration to livestock ls tissue concentration [$\mathrm{kg}_{\text{water}}$/a] and is given by Equation (5-107);
$r^{C14/C12,l}_{lw}(t)$	is the C-14/C-12 ratio in the livestock water for lifestyle l [Bq/$\mathrm{kg}_{\mathrm{C12}}$] given by Equation (5-108);
C^{C12}_{msw}	is the C-12 concentration in the main surface water [$\mathrm{kg}_{\mathrm{C12}}$/$\mathrm{kg}_{\text{water}}$];
C^{C12}_{ls}	is the C-12 concentration in livestock ls tissue [$\mathrm{kg}_{\mathrm{C12}}$/$\mathrm{kg}_{\text{livestock-fw}}$]; and
$R^{C12,ls}_{ing}$	is the C-12 ingestion rate for livestock ls [$\mathrm{kg}_{\mathrm{C12}}$/a] given by Equation (5-109).

The C-14 specific activity transfer parameter for plant concentration to livestock tissue concentration is given by:

$$\mathrm{P}^{C14,\mathrm{ls}}_{\mathrm{p,sa}} = \frac{\mathrm{f}_{\mathrm{feed}} \cdot \mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,feed}} \cdot \mathrm{e}^{-\lambda_{C14} \cdot \mathrm{t}_h}}{\mathrm{DW}_{\mathrm{p}}} \tag{5-106}$$

where,

$\mathrm{P}^{C14,\mathrm{ls}}_{\mathrm{p,sa}}$	is the transfer parameter for plant concentration to livestock ls tissue concentration for C14 [$\mathrm{kg}_{\text{plant-fw}}$/a];
$\mathrm{f}_{\mathrm{feed}}$	is the fraction of feed from contaminated source [-];
$\mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,feed}}$	is the livestock ls ingestion rate of feed [$\mathrm{kg}_{\text{plant-dw}}$/a];
λ_{C14}	is the radioactive decay constant of C-14 [1/a];
t_h	is the hold-up time between plant exposure to contamination and feeding [a]; and
DW_{p}	is the dry/fresh weight ratio for plant p [$\mathrm{kg}_{\text{plant-dw}}$/$\mathrm{kg}_{\text{plant-fw}}$].

The C-14 specific activity transfer parameter for domestic water concentration to livestock tissue is given by:

$$\mathrm{P}^{\mathrm{ls}}_{\mathrm{dom,sa}} = f_w \cdot \mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,wat}} \tag{5-107}$$

where,

$\mathrm{P}^{\mathrm{ls}}_{\mathrm{dom,sa}}$	is the transfer parameter for domestic water concentration to livestock ls tissue concentration [$\mathrm{kg}_{\text{water}}$/a];
f_w	is the fraction of water from contaminated sources [-]; and
$\mathrm{R}^{\mathrm{ls}}_{\mathrm{ing,wat}}$	is the livestock ls ingestion rate of water [$\mathrm{kg}_{\text{water}}$/a].

The C-14/C-12 ratio in the livestock water and is equivalent to Equation (5-19) and is given by:

$$\begin{aligned} r^{C14,\mathrm{l}}_{lw}(t) = {} & \mathrm{f}^{l}_{\mathrm{dom+ls,well}} \frac{\mathrm{C}^{\mathrm{C14,l}}_{\mathrm{well,r}}(t) \cdot f^{C14}_{mol-Bq}}{C^{C12}_{well,r}} \\ & + \left(1 - \mathrm{f}^{l}_{\mathrm{dom+ls,well}}\right) \frac{\mathrm{C}^{C14,\mathrm{l}}_{msw}(t) \cdot f^{C14}_{mol-Bq}}{C^{C12}_{msw}} \end{aligned} \tag{5-108}$$

where,

$r_{lw}^{C14/C12,l}(t)$	is the ratio of C-14 to C-12 in the domestic water for lifestyle l [Bq/kg$_{C12}$];
$C_{well,r}^{C14,l}(t)$	is the concentration of C-14 in the residential well for lifestyle l [mol/kg$_{water}$] given by Equation (5-1);
$C_{msw}^{C14,l}(t)$	is the concentration of C14 in the main surface waterbody [mol/kg$_{water}$] given by Equation (5-16);
C_{well}^{C12}	is the concentration of C-12 in the well water [kg$_{C12}$/kg$_{water}$];
C_{msw}^{C12}	is the concentration of C-12 in the main surface waterbody [kg$_{C12}$/kg$_{water}$];
$f_{dom+ls,well}^{l}$	is the fraction of domestic water that is sourced from the residential well [-] for lifestyle l defined in Equation (5-11); and
f_{mol-Bq}^{C14}	is a conversion factor from moles to Bq for C-14 [Bq/mol].

The C-12 ingestion rate for livestock is given by:

$$R_{ing}^{C12,ls} = \frac{R_{ing,feed}^{ls}}{\mathrm{DW_p}} \cdot C_p^{C12} + R_{ing,wat}^{ls} \cdot C_{lw}^{C12} \qquad (5\text{-}109)$$

where,

$R_{ing}^{C12,ls}$	is the C-12 ingestion rate for livestock ls [kg$_{C12}$/a];
$\mathrm{R_{ing,feed}^{ls}}$	is the livestock ls ingestion rate of feed plants [kg$_{plant\text{-}dw}$/a];
$\mathrm{DW_p}$	is the dry/fresh weight ratio for plant p [kg$_{plant\text{-}dw}$/kg$_{plant\text{-}fw}$].
C_p^{C12}	is the C-12 concentration in plant type p [kg$_{C12}$/kg$_{plant\text{-}fw}$].
$\mathrm{R_{ing,wat}^{ls}}$	is the livestock ls ingestion rate of water [kg$_{water}$/a]; and
C_{lw}^{C12}	is the C-12 concentration in the livestock water [kg$_{C12}$/kg$_{water}$];

5.2.14.2.7 C-14 Specific Activity Wildlife Concentration

The C-14 specific activity wildlife concentration in the biosphere model includes C-14 from ingestion of plants and aquatic biota as well as drinking water. Similar to livestock, ingestion of sediments and soil as well as inhalation are excluded as they are not a significant source of C-14. The C-14 specific activity wildlife concentration due to ingestion of plants, aquatic biota and water is given by:

$$C_{wl,sa}^{C14,l}(\mathrm{t}) = \left(\mathrm{P_{p,sa}^{C14,wl}} \mathrm{C_{p,sa}^{C14,l}}(\mathrm{t}) + \mathrm{P}_{ab,sa}^{\mathrm{wl}} C_{ab,sa}^{C14}(\mathrm{t}) + \mathrm{P}_{\mathrm{dom,sa}}^{wl} r_{msw}^{C14/C12,l}(t) C_{msw}^{C12}\right) \frac{C_{wl}^{C12}}{R_{ing}^{C12,wl}} \qquad (5\text{-}110)$$

where,

$C_{wl,sa}^{C14,l}(\mathrm{t})$	is the C-14 specific activity concentration in wildlife wl for lifestyle l [Bq/kg$_{wildlife\text{-}fw}$] and is equivalent to the wildlife concentration for other radionuclides given by Equation (5-76);
$\mathrm{P_{p,sa}^{C14,wl}}$	is the C-14 specific activity transfer parameter for plant concentration to wildlife tissue concentration for wildlife wl and plant p [kg$_{plant\text{-}fw}$/a] and is given by Equation (5-106) with the indexing superscript “ls” replaced by “wl”;
$\mathrm{C_{p,sa}^{C14,l}}(\mathrm{t})$	is the C-14 specific activity concentration in forage feed plants in lifestyle l [Bq/kg$_{plant}$];

$P_{ab,sa}^{wl}$	is the C-14 specific activity transfer parameter for aquatic biota to wildlife tissue [$kg_{ab\text{-}fw}$/a] and is given by Equation (5-111);
$C_{ab,sa}^{C14}(t)$	is the C-14 specific activity concentration in aquatic biota ab [Bq/$kg_{ab\text{-}fw}$] given by Equation (5-103);
$P_{dom,sa}^{wl}$	is the C-14 specific activity transfer parameter for domestic water concentration to wildlife wl tissue concentration [kg_{water}/a] and is given by Equation (5-107) with the indexing superscript “ls” replaced by “wl”;
$r_{msw}^{C14/C12,l}(t)$	is the C-14/C-12 ratio in the main surface waterbody for lifestyle l [Bq/kg_{C12}] given by Equation (5-104);
C_{msw}^{C12}	is the C-12 concentration in the main surface water [kg_{C12}/kg_{water}];
C_{wl}^{C12}	is the C-12 concentration in wildlife wl tissue [kg_{C12}/$kg_{wildlife\text{-}fw}$]; and
$R_{ing}^{C12,wl}$	is the C-12 ingestion rate for wildlife [kg_{C12}/a] given by Equation (5-112).

The C-14 specific activity transfer parameter for aquatic biota concentration to wildlife tissue is given by:

$$P_{ab,sa}^{wl} = \frac{f_{ab} \cdot R_{ing,ab}^{wl} \cdot f_{ing,ab}^{wl}}{DW_{ab}} \tag{5-111}$$

where,

$P_{ab,sa}^{wl}$	is the transfer parameter for aquatic biota to wildlife tissue [$kg_{ab\text{-}fw}$/a];
f_{ab}	is the fraction of aquatic biota ab from contaminated sources [-];
$R_{ing,ab}^{wl}$	is the wildlife ingestion rate of aquatic biota ab [$kg_{ab\text{-}dw}$/a];
$f_{ing,ab}^{wl}$	is the fraction of each aquatic biota in the wildlife’s wl diet [-]; and
DW_{ab}	is the dry/fresh weight ratio of aquatic biota ab [$kg_{ab\text{-}dw}$/$kg_{ab\text{-}fw}$].

The C-12 ingestion rate for wildlife is given by:

$$R_{ing}^{C12,wl} = \frac{R_{ing,p}^{wl}}{DW_p} \cdot C_p^{C12} + \frac{R_{ing,ab}^{wl} \cdot f_{ing,ab}^{wl}}{DW_p} \cdot C_{ab}^{C12} + R_{ing,wat}^{ls} \cdot C_{msw}^{C12} \tag{5-112}$$

where,

$R_{ing}^{C12,wl}$	is the C-12 ingestion rate for wildlife wl [kg_{C12}/a];
$R_{ing,p}^{wl}$	is the wildlife ingestion rate of plant p [$kg_{plant\text{-}dw}$/a];
DW_p	is the dry/fresh weight ratio for plant p [$kg_{plant\text{-}dw}$/$kg_{plant\text{-}fw}$].
C_p^{C12}	is the C-12 concentration in plant type p [kg_{C12}/$kg_{plant\text{-}fw}$];
$R_{ing,ab}^{wl}$	is the wildlife ingestion rate of aquatic biota ab [$kg_{ab\text{-}dw}$/a];
$f_{ing,ab}^{wl}$	is the fraction of each aquatic biota in the wildlife’s wl diet [-];
DW_{ab}	is the dry/fresh weight ratio of aquatic biota ab [$kg_{ab\text{-}dw}$/$kg_{ab\text{-}fw}$].
C_{ab}^{C12}	is the C-12 concentration in aquatic biota type ab [kg_{C12}/$kg_{ab\text{-}fw}$].
$R_{ing,wat}^{wl}$	is the wildlife wl ingestion rate of water [kg_{water}/a]; and
C_{msw}^{C12}	is the C-12 concentration in the main surface water [kg_{C12}/kg_{water}].

5.2.14.2.8 C-14 Specific Activity Doses

The C-14 specific activity model only affects the C-14 concentration in biosphere compartments and components. The C-14 specific activity dose is calculated as described in the dose model theory (Section 5.2.13).

5.2.15 Element Concentration in Environmental Media

For each of the media (surface soil, surface water, well, sediment, and air), the concentration of each element is determined by summing the contribution of all isotopes j of each element k and is given by:

$$\mathrm{C}_{\mathrm{m}}^{\mathrm{k,l}}(\mathrm{t}) = \sum_{\mathrm{k} \in \mathrm{j}} \mathrm{C}_{\mathrm{m}}^{\mathrm{j,l}}(\mathrm{t}) \qquad (5\text{-}113)$$

where,

$\mathrm{C}_{\mathrm{m}}^{\mathrm{k,l}}(\mathrm{t})$ is the concentration in medium m of element k for lifestyle l [mol/m^3 or mol/kg]; and

$\mathrm{C}_{\mathrm{m}}^{\mathrm{j,l}}(\mathrm{t})$ is the concentration in medium m of radionuclide j for lifestyle l [mol/m3 or mol/kg].

When multiple media of a given type (e.g., multiple surface waters) are considered, the highest surface water concentration is typically used for comparison with environmental media concentration limits.

5.3 Revell Site Biosphere Model

The ISM-BIO model estimates the potential environmental and health impacts of a deep geologic repository in the long term after the closure of the repository, in a temperate climate state at the Revell site. It estimates the consequences to several hypothetical receptors (or lifestyles) that might live at the site in the future, as an indicator of the health and environmental consequences of any release from the geosphere.

The ISM-BIO model is a simplified representation of the Revell biosphere. The biosphere is represented by 12 different biosphere compartments, 10 biosphere components and 17 exposure pathways. Compartments include surface waters and soils. Contaminants transferred between compartments represent migration from one compartment to the next via a defined transfer rate. Components represent features in the biosphere whose concentration is estimated assuming an equilibrium with a specific biosphere compartment or component. Examples of components in the biosphere include sediments, plants and animals.

Figure 5-7 shows the connection between ISM-BIO model compartments and Figure 5-8 shows the connection between the ISM-BIO compartments and components including environmental media and biota. The well is included as a source applied to both compartments and components. Note that a sink is included as a compartment. This represents loss from the local biosphere due to processes like outflow, burial into sediments and volatilization.

Concentration of elements in the compartments and components are compared with relevant criteria for chemical toxicity. Concentration of radionuclides in the compartments and components are used to estimate dose consequences to humans assumed to be living at the repository site via defined dose pathways.

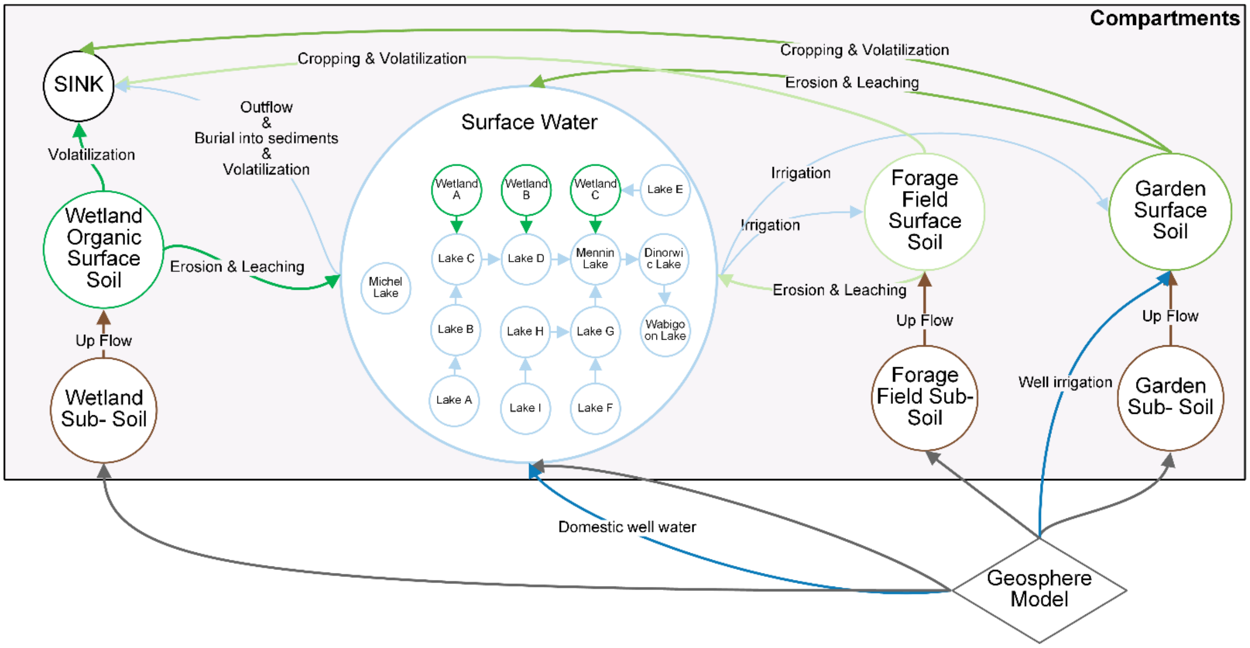

Figure 5-7: Contaminant Transport Model Biosphere Compartments for ISM-BIO Model of the Revell Site

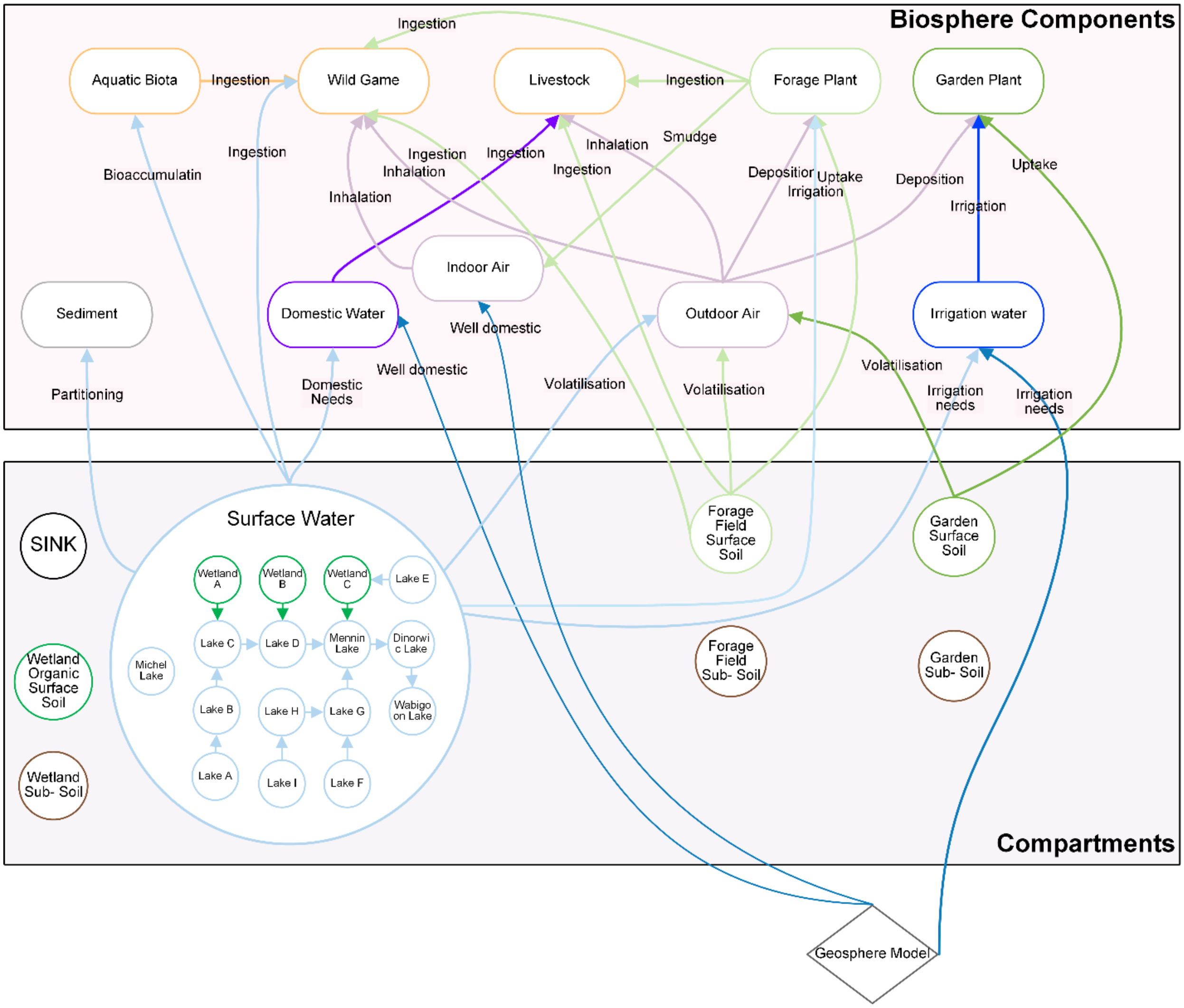

Figure 5-8: Contaminant Transport Model Compartments and Components for ISM-BIO Model of the Revell Site

Dose pathways included in the ISM-BIO model are shown in Figure 5-9. Dose pathways depend on the lifestyle of the individuals assumed to be living above or near the repository. The ISM-BIO model evaluates the consequences for several different illustrative lifestyles through sequential model runs. For example, one lifestyle is intended to represent a maximally-exposed group and is based on human behaviour using conservative assumptions from CSA (2020). Additional illustrative lifestyles are intended to be broadly representative of local residents of the Revell area (e.g., a town resident, a rural resident or member of a local first nations community) and are based on current human behaviours.

Three age groups (adults, children and infants) are assessed for the maximally-exposed lifestyle whereas only adults are assessed for the other lifestyles. The biosphere model theory (Section 5.2) presents the theory for all potential exposure pathways. Lifestyles and ages are differentiated through input parameters that determine if a pathway is active for a given lifestyle and age group.

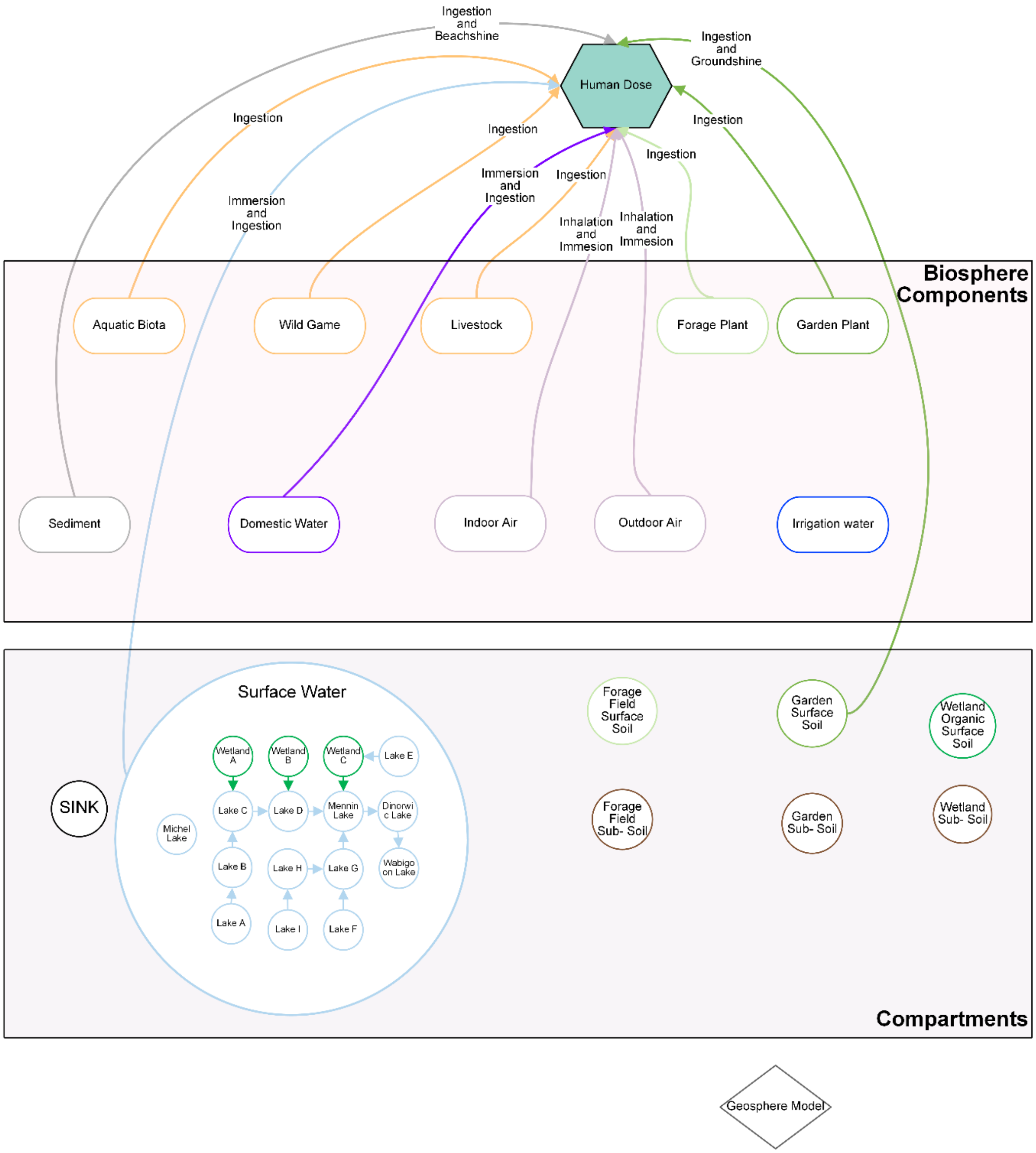

Figure 5-9: ISM-BIO Dose Pathways for the Revell Site

Wetland can also be converted to farmlands (garden field) in the ISM-BIO model (Section 5.2.9). The modified conceptual model for ISM-BIO is presented in Figure 5-10 and Figure 5-11.

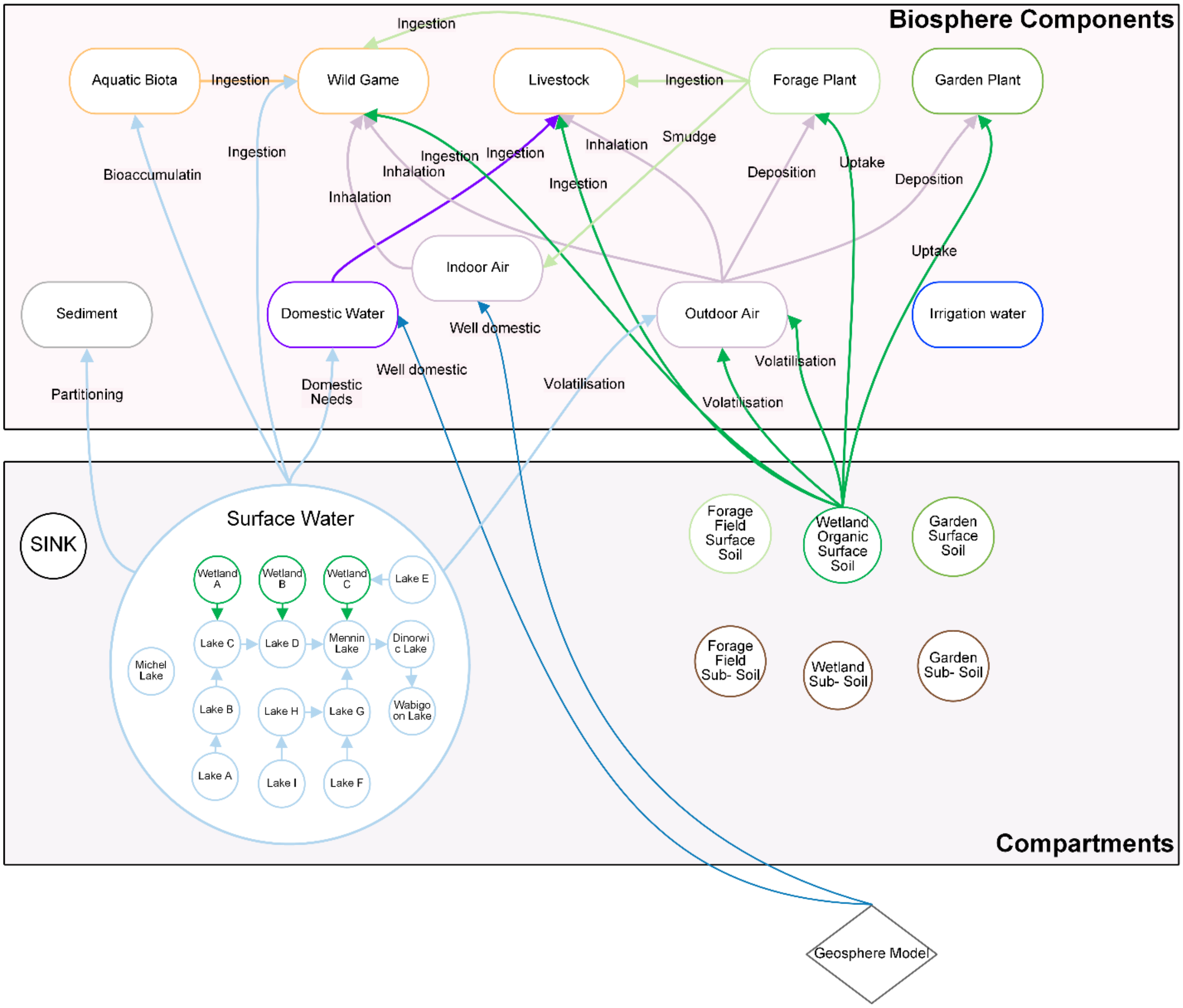

Figure 5-10: ISM-BIO Compartments and Compartments – Wetland Sensitivity

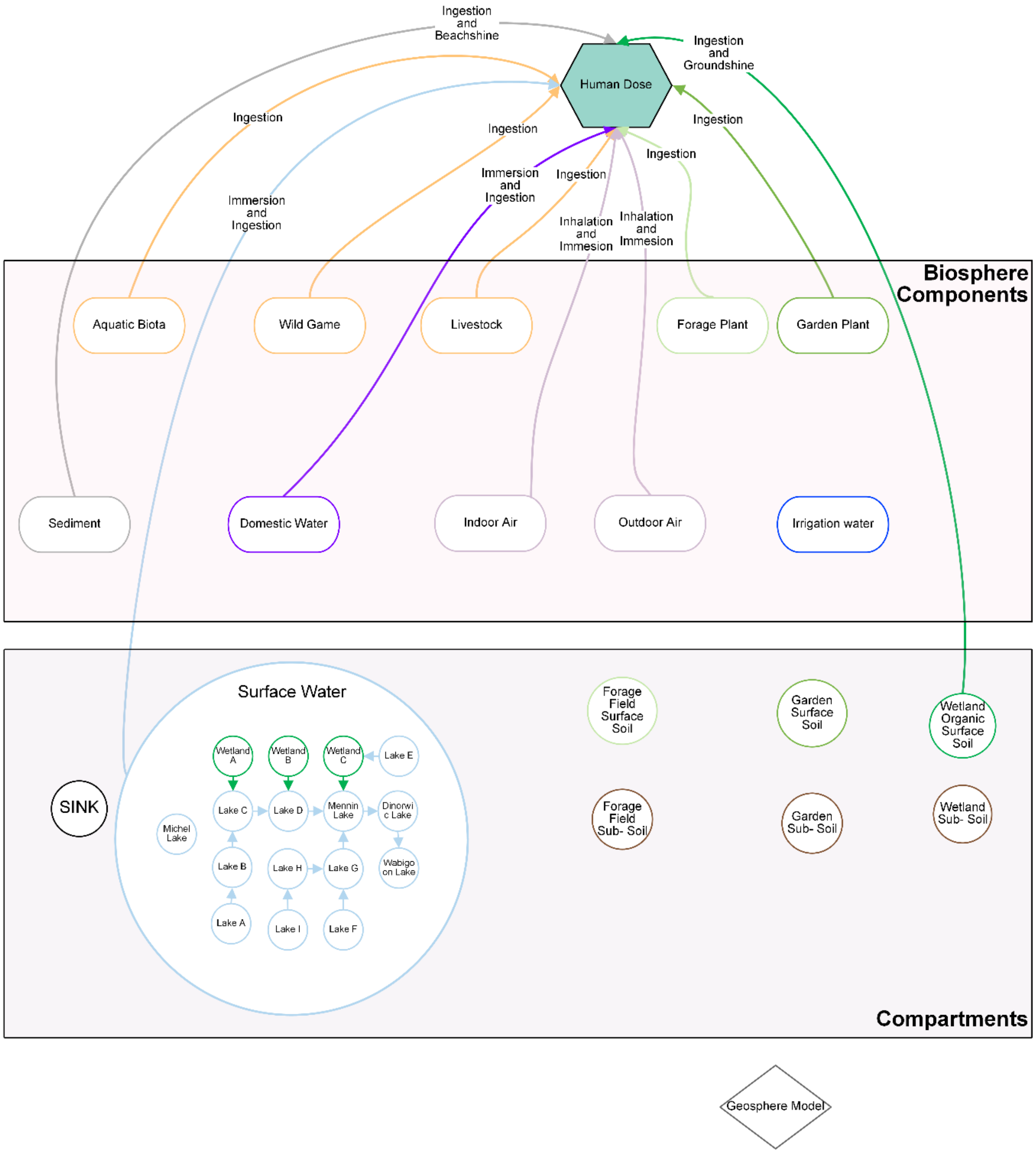

Figure 5-11: ISM-BIO Exposure Pathways – Wetland Sensitivity

For the C-14 specific activity model (Section 5.2.14.2) the connection between the biosphere compartments, components and the dose model are somewhat different than those in those shown in Figure 5-7 through Figure 5-9. The connection between the biosphere compartments, components in the C-14 specific activity dose model are shown in Figure 5-12.

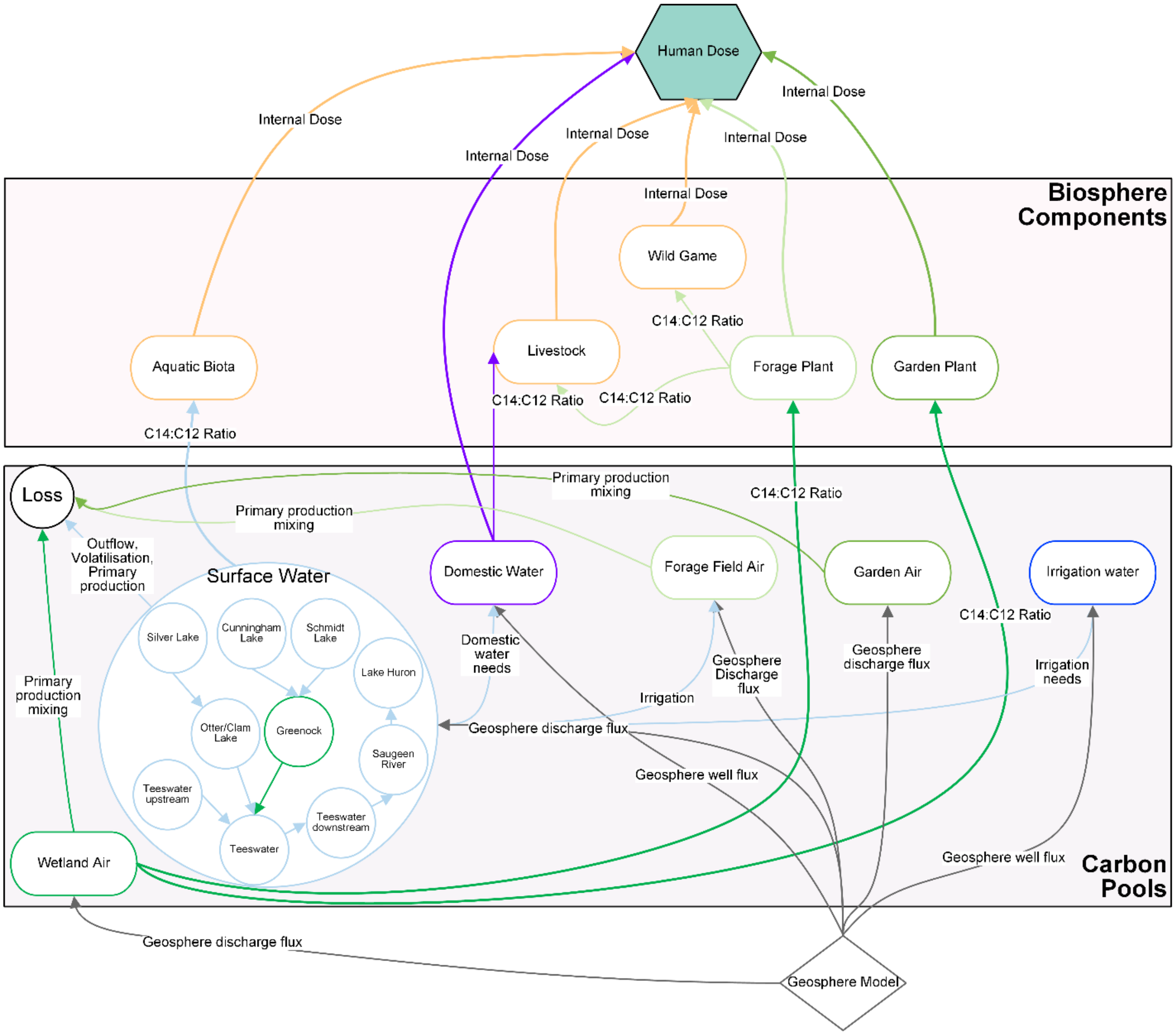

Figure 5-12: ISM-BIO C-14 Specific Activity Conceptual Model

6. SUMMARY

This report describes the theory for the Integrated System Model (ISM). The ISM is a system model designed to assess the transport of elements and radionuclides and to calculate the doses and concentrations of chemically toxic elements in the biosphere, for post-closure safety assessments of a deep geologic repository for used nuclear fuel. The system model is composed of a series of linked models representing the wasteform (ISM-WF), the geosphere (ISM-GEO) and the biosphere (ISM-BIO).

The present document is applicable to ISM v1.4. Significant changes to the ISM v1.4 relative to v1.3 are described below. Details on changes between historical versions are provided in Appendix B.

<u>ISM</u>

- Retired versions of the ISM models representing the South Bruce Site following the site selection decision and removed South Bruce related content from the ISM theory manual. No changes were made to the ISM-GEO and ISM-BIO models representing the Revell Site.

<u>ISM-NF</u>

- ISM-NF becomes an optional component of ISM v1.4 (model overview and theory moved to Appendix A).

<u>ISM-WF</u>

- Development of a new wasteform model (ISM-WF). The ISM-WF model is used to estimate radionuclide and element “source terms” from a variety of wasteforms that may be disposed of in the DGR (e.g., CANDU fuels, prototype fuels, research fuels, and low-level wastes).

7. FUTURE DEVELOPMENT

This iteration of the ISM is informed by some initial preliminary characterization of the Revell Site. However, many of the NWMO site characterization programs and supporting modelling are in their early stages. Consequently, much of the current ISM theory remains somewhat generic.

The ISM will continue to be iterated as the NWMO detailed site characterization programs advance. Future versions of the ISM will be informed by the evolution of the repository design, site characterization programs (environmental and geoscientific), complementary computer modelling programs, as well as site-specific features, events and processes.

Future iterations of the ISM will also be informed by the review or feedback from key stakeholders and expert reviewers and well as the iterative safety assessment process.

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APPENDIX A – NEARFIELD MODEL

The near-field model (also referred to as the ISM-NF model) consists of the fuel (not explicitly represented), engineered barrier system, excavation damaged zone and intact host rock surrounding the placement room and the processes therein. The near-field model geometry (Figure A-1, Figure A-2) includes a representation the container, the engineered barrier system (Highly Compacted Bentonite or HCB, buffer boxes and spacer blocks, bentonite gap fill and concrete floor), inner and outer excavation damaged zones (EDZ) and host rock. Several assumptions simplifying the near-field model geometry have been made in order to reduce execution time of the model. The simplifying assumptions and rationale are provided in Table A-1.

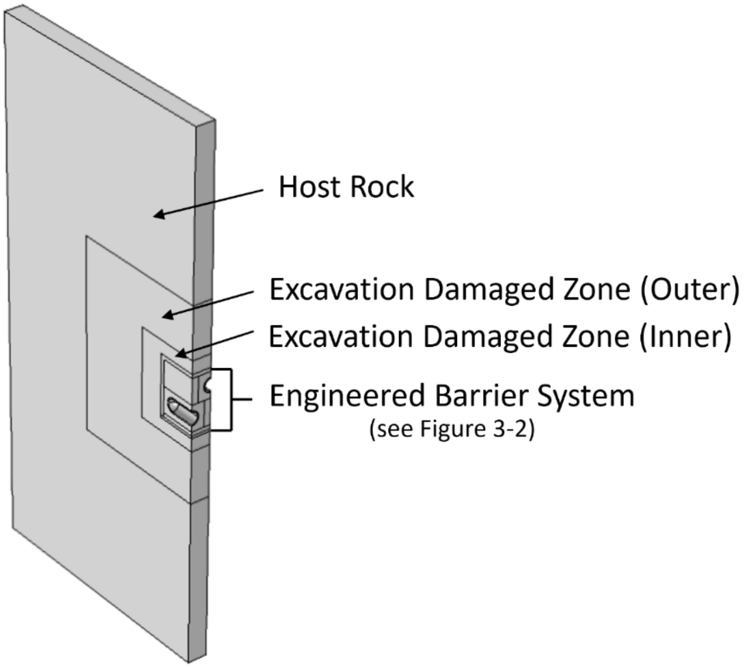


Figure A-1: Near-Field Model Geometry (Model Extents)

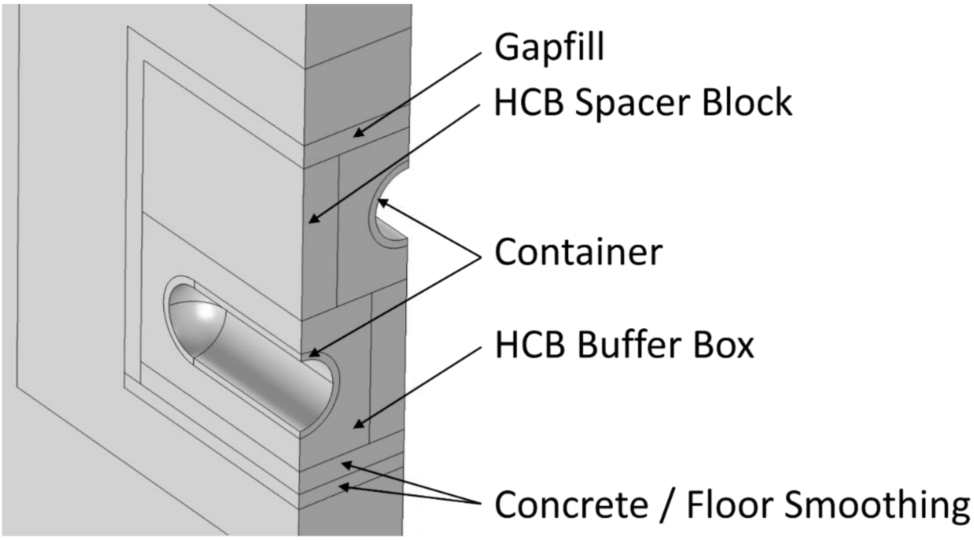


Figure A-2: Near-field Model Geometry (Engineered Barrier System)

Table A-1: Simplifying ISM-NF Geometry Assumptions and Rationale

Simplifying Geometric Assumption	Discussion and Rationale
Fuel and interior components of the container are not explicitly represented in the ISM-NF model	- Fuel and zircaloy surface areas accounted for in the fuel and zircaloy dissolution models (see Sections A.1.3 and Section A.1.7). - Inclusion of fuel, container baskets and other container components would inhibit transport from the container and therefore excluding these components is conservative.
Reduced detail of placement room components (e.g., omission of lookouts, rectangular placement rooms)	- Lookouts represent additional transport length of 0.15 m to 0.25 m based on current preliminary repository designs. ISM-NF model assumes minimum placement room width and is therefore conservative. - Small gaps (e.g., between HCB blocks) are expected to be filled by swelling of the bentonite (HCB and gap fill) as the repository resaturates. - The placement room design is subject to change and the near-field model, although somewhat abstracted is sufficiently representative of the current design.
Planar symmetry is used	- Utilizing planar symmetry in 3D modelling is a common and widely accepted approach to reduce model size and complexity (see Section A.3).
A small segment of the placement room (two quarter containers) is represented	- ISM-NF assumes contributions from other failed containers is additive. - Other nearby failed containers would reduce the concentration gradient across the placement room and result in a reduced overall release from placement room (except at the ends of the placement rooms).

A.1 Near-field Model Overview

The repository concept is designed to isolate and contain radioactive wastes essentially indefinitely. However, the ISM is a post-closure safety assessment model, which considers the consequence of failed containers. In the ISM, potential failure processes (e.g., corrosion) are not modelled. Instead, the initial time of failure (or delay time) is provided as a model input. Once failed it is assumed that the water has filled the container and is in contact with the fuel. The near-field model can be divided into the conceptual wasteform model, and the 3D placement room model (engineered barrier system, excavation damaged zone and host rock) in terms of processes considered. The near-field model includes the following processes:

- Decay and ingrowth of contaminants in the fuel (see Section 2.4)
- Instant release of a fraction of the fuel contaminant inventory (Section A.1.2)
- Radiolysis and chemical degradation of the fuel matrix (Section A.1.3)
- Instant release of a fraction of the Zircaloy inventory upon failure of the container (Section A.1.6);
- Corrosion degradation of the Zircaloy (Section A.1.7);

- Solubility limited release of contaminants that exceed defined solubility limits (Section A.1.9); and
- Transport via diffusion and advection (with sorption) of dissolved contaminants through the engineered barrier system, the excavation damaged zone and into the intact host rock (Section A.2.5).

The conceptual near-field model makes a number of assumptions regarding the processes included in the model. These assumptions and their rationale are included in Table A-2.

The output of the near-field model is time dependent transport (typically in mol/a, Bq/a or kg/s) of contaminants entering the geosphere. Transport to the geosphere is calculated by integrating the flux through one of a few predefined interfaces in the near-field model. For example, the interface between the container and the bentonite or the outer excavation damage zone (EDZ) and the intact rock (see Section A.4). This output from the near-field model is used as a source term in the geosphere model.

Table A-2: Simplifying ISM-NF Conceptual Assumptions and Rationale

Simplifying Conceptual Assumption	Discussion and Rationale
The near-field is assumed to be fully saturated at the time of container failure and all model features are treated as saturated porous media.	- Liquid-mediated transport of contaminants from the container to the geosphere is expected to be much slower under partially saturated conditions due to the reduction in accessible porosity. - Time of container failure (input parameter) can account for resaturation time.
Fuel surface area is assumed to be constant in the radiolysis fuel dissolution model (Section A.1.5)	- Fuel surface area (parameter value) can be selected consider various fuel states (generally assumed to be heavily fractured). - As fuel dissolves it is expected that the fuel surface area will decrease over long periods of time. It is therefore conservative (albeit somewhat unrealistic) to assume a constant fuel surface area.
Cladding surface area is assumed to be constant in the cladding congruent release model (Section A.1.7)	- Most radionuclides are expected to be trapped within the oxide layer of the cladding. - The cladding is thin and formed in layers or sheets which will decrease with time however significant increases or decreases in surface area are not expected to occur over time.
The effect of the Zircaloy cladding on delaying or inhibiting fuel corrosion is ignored.	- Intact Zircaloy cladding will prevent water from accessing the fuel pellets. - If damaged the cladding may not inhibit water's ability to access to the fuel pellets. - It is conservatively assumed that the cladding does not inhibit water access to the fuel once the container fails. - Cladding damage or failure processes are not modelled.
Containers are assumed to retain their general integrity such that the	- Internal components of the container (e.g., fuel baskets) are not modelled and the inside of the

Simplifying Conceptual Assumption	Discussion and Rationale
container internal volume is not reduced even when failed.	container is treated as a well-mixed compartment. - Including build-up of corrosion products or ingress of bentonite into the container would inhibit the release of contaminants from the container. - Source terms are applied to the surface of the container or the volume representing the container shell (see Section A.1.8) i.e., minimal transport distance to the bentonite.
The build-up of steel corrosion products within the container or migration of bentonite into the container is not modelled.	- Corrosion products or bentonite ingress into the container would fill void spaces in the container and reduce the available porosity in the container. They could also provide additional materials for sorption to occur. Decreasing transport from the container to the geosphere - Fe^{2+} and H_2 will compete for radiolytic oxidants (primarily H_2O_2) responsible for fuel dissolution; including corrosion in the modelling would reduce the assumed fuel dissolution rate.
The container interior is treated as a well mixed volume of water and sorption is neglected.	- Conservative assumption as explicitly representing fuel, internal components of the container (e.g., baskets), corrosion products and sorption onto these materials would inhibit transport out of the container.
Solubility of radionuclides are only limited within the container	- Solubilities of species are limited within the container and species that exceed the solubility limit will precipitate. - Solubilities are not limited beyond the container as concentrations are generally expected to be higher in the container (e.g., precipitation resulting from ingrowth in the bentonite is ignored) - Coprecipitation of isotopes of the same element is considered. - Coprecipitation of chemically similar elements is not considered.
Advective velocities are not computed. Unique velocities (magnitude and direction) can be input for each model domain (e.g., Concrete, HCB, Gap fill, EDZ, rock).	- Advection strongly depends the hydrogeological conditions local to the placement room and the condition of the engineered sealing materials. - Accurately determining advective flow fields in the ISM-NF alone is not possible and they are therefore input and based on a larger scale model (e.g., ISM-GEO).
A linear equilibrium sorption (kd) model is assumed in the near-field model. Unique sorption coefficients can be applied to each model domain	- Linear equilibrium sorption is applicable at low concentrations which should be relevant to most radionuclides.

Simplifying Conceptual Assumption	Discussion and Rationale
(e.g., Concrete, HCB, Gap fill, EDZ, rock).	
Material properties (e.g., porosity, density) within container interior, engineered barrier system (HCB, gap fill), and excavation damaged zones are assumed to be homogeneous and constant.	- The near-field is designed to be relatively homogenous in placed materials. - It is anticipated that HCB will tend to equilibrate to near uniform conditions over time. - It is also anticipated that gap fill will tend to equilibrate to uniform conditions over time (distinct from HCB)
Formation and transport of colloids are not modelled.	- It is assumed that natural groundwater colloids are not significant at Revell site based on general expectations for deep porewaters. - Colloids may form by corrosion and degradation processes occurring within and around the containers; however, they are unable to pass through the buffer due to its pore structure. - Precipitation could form intrinsic colloids, but they are retained inside the buffer.

A.1.1 Wasteform

The current reference wasteform is a 37R CANDU used fuel bundle, consisting of irradiated UO_2 encased in Zircaloy cladding (Figure A-3). As discussed in Section 2.1 other fuel types and wasteforms may be considered.

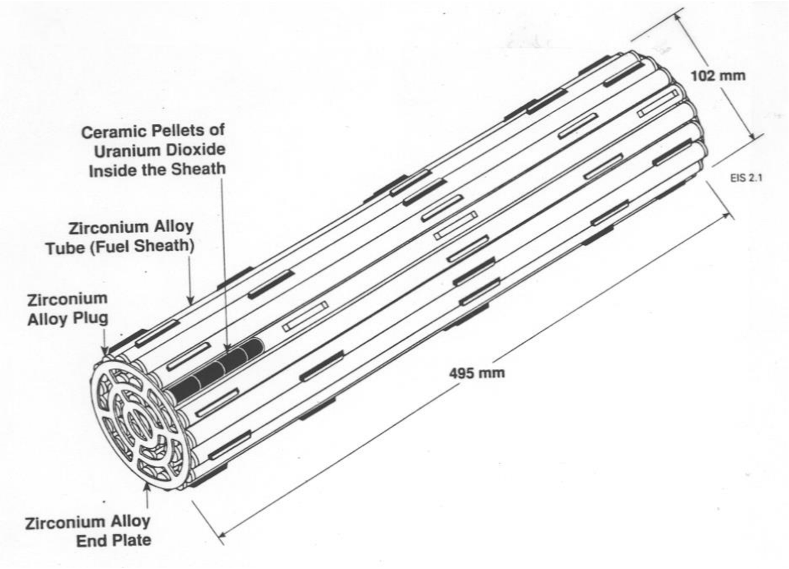


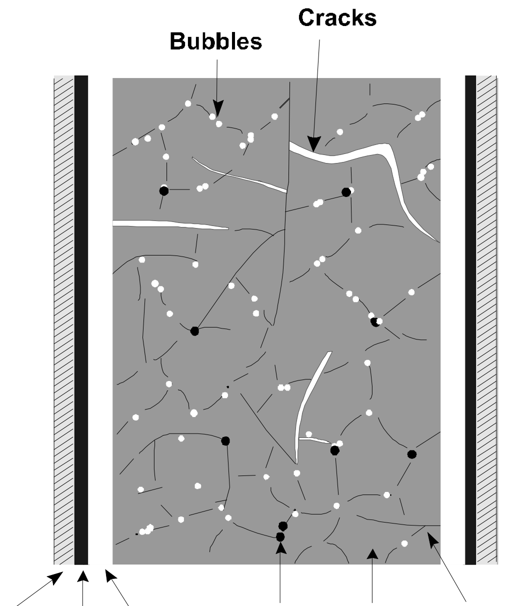
Figure A-3: CANDU Fuel Bundle

In the ISM-NF model the fuel geometry is not explicitly represented so geometric differences in fuels or wasteforms are not realized (see Figure A-2). However, the fuel and Zircaloy surface areas are accounted for in the fuel dissolution model (see Sections A.1.3 and Section A.1.7). Variations in the fuel type, composition, burnup and power can be captured via the inventory of contaminants in the fuel and other fuel dissolution model parameters.

The wasteform model includes releases from the UO_2 fuel matrix and the Zircaloy cladding. The detailed wasteform model theory is described in Section A.1.2 through A.1.8. Note that other wasteforms may be analyzed with the appropriate inventory and fuel degradation input parameters.

A.1.2 Instant Release from UO_2 Matrix

The radionuclides and stable elements within the UO_2 fuel pellet are distributed among various locations by the end of the reactor irradiation, as illustrated in Figure A-4 (Johnson et al. 1994). While the bulk of the radionuclides are held within the UO_2 grains, certain metals have formed metallic particulates, and the balance (notably the more volatile contaminants) have collected in grain boundaries, cracks, and external gaps around the fuel. When the cladding is breached and the fuel is contacted by water, the location of the nuclides affects the rate at which they are released into the groundwater.



Zircaloy Cladding	CANLUB	Gap	Metal Particles	UO_2 Matrix	Grain Boundary
^{14}C ^{59}Ni	^{14}C ^{129}I ^{135}Cs ^{79}Se ^{125}Sn ^{3}H ^{39}Ar ^{4}He ^{85}Kr	^{14}C ^{129}I ^{135}Cs ^{79}Se ^{99}Tc ^{125}Sn ^{3}H ^{39}Ar ^{4}He ^{85}Kr	Mo Ru Pd Rh Tc	Actinides ~98% Fission Products	^{14}C ^{129}I

Figure A-4: Distribution of Various Radionuclides within a Used Fuel Element

In particular, rapid release and slow release processes are defined. The rapid or “instant” release applies to all nuclides within the gaps, cracks and grain boundaries, which are assumed to be quickly accessed by water and dissolved. The slow release applies to all nuclides within the grains and the intermetallic particles, which are only released as the UO_2 grains themselves dissolve. The latter mechanism is referred to as “congruent” release and is described in Section A.1.3.

The rate of release of contaminant j from the UO_2 matrix by instant release is given by Equation (A-1) which is based on Equation 2.67 from NWMO (2012). Rather than a delta function as described in NWMO (2012) the UO_2 instant release in the ISM-NF model occurs via a smoothed (numerically stable) rectangular function at the time of container failure.

$$F^{j}_{IRF,UO2}(t) = \frac{f^{j}_{IRF,UO2} I^{j}_{UO2}(t)\delta(t_F, t_{IRF})}{N_{Symmetry}} \tag{A-1}$$

where,

$F^{j}_{IRF,UO2}(t)$	is the UO_2 rapid or “instant” release rate of contaminant j entering the water filled void in the container [mol/a];
$f^{j}_{IRF,UO2}$	is the fraction of contaminant j release instantly from the UO_2 matrix upon contact with water [-];
$I^{j}_{UO2}(t)$	is the inventory of contaminant j at time t in the UO_2 fuel in a container [mol];
$\delta(t_F, t_{IRF})$	is a rectangular function occurring at t_F and having a width of t_{IRF} [1/a];
t_F	is the time of container [a] defined by Equation (A-2);
t_{IRF}	is the time over which the instant release is assumed to occur [a]; and
$N_{Symmetry}$	is the scaling from a fractional container to a whole container. For a single quarter section of a container $N_{Symetry}$ is 4.

$$t_F = \min\,(t_b, t_h) \tag{A-2}$$

where,

t_b	is the failure time of the container body [a];
t_h	is the failure time of the container hemi-head [a];

A.1.3 Congruent Release from the Fuel Matrix

The UO_2 ceramic fuel matrix is durable and dissolves slowly in water. The most important factor in the rate of dissolution of UO_2 are the redox conditions established in the groundwater within the failed container (Shoesmith et al. 1997, Badley and Shoesmith 2022). Prior to container failure, reducing conditions will be rapidly established around the container after emplacement in a repository due to the consumption of any residual oxygen by reaction with either the copper and steel container materials or with ferrous and organic materials in the bentonite sealing materials. Thus, the only available source of oxidants at the fuel surface would be radiolysis of the groundwater within the failed container, with reducing redox conditions re-established by the production of hydrogen both radiolytically and by corrosion of the steel container (Badley and Shoesmith, 2022). Under these conditions, the UO_2 would dissolve very slowly.

A.1.4 Fractional Fuel Dissolution Model

Badley and Shoesmith (2022) show that the threshold below which there is no observable effect of alpha activity on fuel dissolution is between 1 MBq/gUO_2 and 33 MBq/gUO_2. In the presence of a reducing agent (either H_2 or metallic iron in solution), the threshold is displaced towards higher activity levels, as noted by Muzeau et al. (2009). In the presence of hydrogen (pH_2 = 1 bar) and 1 mM carbonate solution, the threshold rises above 385 MBq/g(UO_2). Similar findings were observed by Fors (2009). For comparison the alpha activity of the reference CANDU fuel bundle is 124 MBq/g(UO_2) when discharged from the reactor. This suggests that even small amounts of dissolved H_2 are sufficient to suppress the fuel dissolution rate below the threshold above which alpha activity has an observable effect on the fuel dissolution rate. Similar conclusions were made by SKB (SKB 2022, Werme et al. 2004), Posiva (Posiva, 2021), and Nagra (Johnson, 2014).

Based on a large amount of data published in open literature (Figure 6 and Section 6.3.18 of Posiva (2021)) for UO_2 dissolution in the presence of hydrogen gas and or corroding iron and iron corrosion products is vanishingly small. In fact, a common finding from leaching studies by several research groups is that it is often impossible to measure an actual dissolution rate in reducing conditions, even in the presence of a sample with a high alpha activity, as the U concentration remains stable (or oscillates) around the solubility limit of UO_2 for long periods of time.

As a result, the NWMO has adopted a fractional fuel dissolution model consistent with the model proposed by SKB (SKB 2022, Werme et al. 2004) and described by Equation (A-3). This approach considers the presence of redox scavengers as described in Badley and Shoesmith (2022) and is conservative relative to current scientific evidence and experiments as noted by SKB (SKB 2022), Posiva (Posiva 2021) and Nagra (Johnson, 2014).

$$F_{CD,UO2}^{j}(t) = \left(1 - f_{IRF,UO2}^{j}\right)\frac{I_{UO2}^{j}(t)}{N_{Symmetry}} C_{frac,UO2}\left(1 - S_{rad/frac}\right)(t \geq t_F)\left(t \leq \frac{1}{C_{frac,UO2}}\right) \quad \text{(A-3)}$$

where,

$F_{CD,UO2}^{j}(t)$	is the UO_2 congruent dissolution rate of contaminant j entering the water filled void in the container [mol/a]
$f_{IRF,UO2}^{i}$	is the fraction of contaminant j release instantly from the UO_2 matrix upon contact with water [-];
$I_{UO2}^{j}(t)$	is the inventory of contaminant j at time t in the UO_2 fuel in a container [mol];
$N_{Symmetry}$	is the scaling from a fractional container to a whole container. For a single quarter section of a container $N_{Symetry}$ is 4.
$C_{frac,UO2}$	is the fractional UO_2 matrix degradation rate [1/a];
$S_{rad/frac}$	is a Boolean switch parameter equal to 1 if the radiolysis fuel dissolution model is used and 0 if the fractional fuel dissolution model is used; and
t_F	is the time of container failure [a] defined by Equation (A-2).

A.1.5 Radiolytic Fuel Dissolution Model

This fuel dissolution model ignores the influence of hydrogen (both radiolytically and by corrosion) and assumes conditions at the used fuel surface could remain oxidizing for a long time due to the production of oxidants near the fuel by radiolysis of water. This water would have reached the fuel only after failure of the container and fuel cladding. Radiolysis of groundwater would be caused by the α, β and γ radiation emitted by the used fuel.

The fuel dissolution in this model is based on an empirical model for radiolysis-driven dissolution. In this approach the rate of fuel dissolution of the used fuel matrix due to α, β and γ radiolysis is modelled by Equation (A-4). The current radiolysis-based fuel dissolution model is based on effective G-values introduced in Johnson and Smith (2000). Effective G-values are derived from experimental data in Johnson et al. (1996) and Badley and Shoesmith (2022).

$$C_{rad,UO2} = \frac{A_{fuel}}{N_{Symmetry}} \left[G_{\alpha} f_{\alpha} D_{\alpha} (t + t_c)^{a\alpha} + G_{\beta} f_{\beta} D_{\beta} (t + t_c)^{a\beta} + G_{\gamma} f_{\gamma} D_{\gamma} (t + t_c)^{a\gamma} + R_{Uchem} \right] \tag{A-4}$$

where,

$C_{rad,UO2}$	is the UO_2 matrix degradation rate in the failed container at time t due to radiolysis [mol/a];
A_{fuel}	is the effective surface area of the dissolving fuel, per container [m^2];
$D_{\alpha}(t + t_c)$	is the time-dependent alpha dose rates [Gy/a];
$D_{\beta}(t + t_c)$	is the time-dependent beta dose rates [Gy/a];
$D_{\gamma}(t + t_c)$	is the time-dependent gamma dose rates [Gy/a];
t	is the time after repository closure [a];
t_c	is the time between fuel removal from reactor and repository closure [a];
G_{α}, G_{β}, G_{γ}	are empirical rate constants for fuel dissolution in the presence of alpha, beta and gamma radiation fields, respectively [$mol_{uo2}/m^2/Gy$];
f_{α}, f_{β}, f_{γ}	are the alpha dose, beta dose, and gamma dose variability factors, accounting for uncertainties in the radiation field strengths due to, for example, uncertainties in the contaminant inventories, and are approximately equal to unity [-].
$a\alpha$, $a\beta$, $a\gamma$	are fitting parameters for the dependence of the fuel dissolution rate on the alpha, beta, and gamma dose rates, and are approximately equal to one [-]; and
R_{Uchem}	is the chemical fuel dissolution rate, i.e., the dissolution rate of the fuel in the absence of radiolysis [$mol_{uo2}/m^2/a$].

The beta/gamma contribution is expected to be dominant for the first 500 years. After this time, the fission products will have largely decayed and most of the remaining radioactivity in the fuel will be due to the actinides. Since actinides tend to decay by alpha decay, at long times alpha radiolysis will control the fuel dissolution rate. H_2 gas generated by corrosion of iron within the container may reduce the effective dissolution rate and can be included via the dissolution rate constants (Badley and Shoesmith 2022).

The congruent dissolution release rate of contaminants j from the UO_2 fuel matrix in the failed container at time *t* is given by Equation (A-5).

$$F^{j}_{CD,UO2}(t) = \left(1 - f^{j}_{IRF,UO2}\right) \frac{I^{j}_{UO2}(t)}{N_{Symmetry}} \frac{C_{rad,UO2}(t)}{I_{0,UO2}} S_{rad/frac}(t \geq t_F)(t \leq t_{UO2}) \tag{A-5}$$

where,

$F^{j}_{CD,UO2}(t)$	is the UO_2 congruent dissolution rate of contaminant j entering the water filled void in the container [mol/a]
$f^{i}_{IRF,UO2}$	is the fraction of contaminant j release instantly from the UO_2 matrix upon contact with water [-];
$I^{j}_{UO2}(t)$	is the inventory of contaminant j at time t in the UO_2 fuel in a container [mol];
$N_{Symmetry}$	is the scaling from a fractional container to a whole container. For a single quarter section of a container $N_{Symetry}$ is 4.
$C_{rad,UO2}(t)$	is the UO_2 matrix degradation rate in the failed container at time t due to radiolysis [mol/a];
$I_{0,UO2}$	is the initial inventory of UO_2 in a container [mol];
$S_{rad/frac}$	is a Boolean switch parameter equal to 1 if the radiolysis fuel dissolution model is used and 0 if the fractional fuel dissolution model is used.

t_F	is the time of container failure [a] defined by Equation (A-2); and
t_{UO2}	is the time all UO_2 has been dissolved [a] (see Equation (3-5)).

The UO_2 degradation rate only applies after a container has failed and continues while some inventory of UO_2 fuel remains in the failed container. The time at which all the UO_2 has been dissolved is determined by calculating the time at which Equation (A-6) has been satisfied.

$$\frac{I_{0,UO2}}{N_{Symmetry}} = \int_{t_F}^{t_{UO_2}} C_{rad,UO2}(t) \tag{A-6}$$

Equation (3-5) is solved numerically as the near-field runs.

A.1.6 Instant Release from the Zircaloy Cladding

Like the UO_2 matrix, rapid release and slow-release processes in the Zircaloy is modelled. The rapid or “instant” release applies to soluble contaminants such as those trapped in the outer surface oxide layer, which are assumed to be released more rapidly. The slow release applies to all contaminants within Zircaloy cladding material that are released as the cladding corrodes. The latter mechanism is referred to as “congruent” release and is described in Section A.1.7.

The rate of release of contaminant j from the Zircaloy cladding by instant release is described by Equation (A-7) which is based on Equation 2.69a from NWMO (2012). Similar to the UO_2 instant release, the Zircaloy instant release occurs via a smoothed rectangular function at the time of container failure in place of the delta function used in NWMO (2012).

$$F^{j}_{IRF,Zr}(t) = \frac{f^{j}_{IRF,Zr} I^{j}_{Zr}(t)\delta(t_F, t_{IRF})}{N_{Symmetry}} \tag{A-7}$$

where,

$F^{j}_{IRF,Zr}(t)$	is the Zircaloy instant release rate of contaminant j entering the water filled void in the container [mol/a];
$f^{j}_{IRF,Zr}$	is the fraction of contaminant j release instantly from the Zircaloy cladding upon contact with water [-];
I^{j}_{Zr}(t)	is the inventory of contaminant j at time t in the Zircaloy cladding in a container [mol];
$\delta(t_{IRF}, t_F)$	is a rectangular function occurring at t_F and having a width of t_{IRF};
t_F	is the time of container failure [a] defined by Equation (A-2); and
t_{IRF}	is the time over which the instant release is assumed to occur [a].
$N_{Symmetry}$	is the scaling from a fractional container to a whole container. For a single quarter section of a container $N_{Symetry}$ is 4.

A.1.7 Congruent Release from Zircaloy Cladding

The Zircaloy sheath surrounding the fuel pellets in a CANDU fuel bundle naturally forms a thin layer of protective ZrO_2 on its surface when in contact with air or water. In the event a container fails, the oxide layer greatly inhibits the Zircaloy dissolution rate (Shoesmith and Zagidulin 2010).

A kinetic dissolution model is used in which the zirconium dissolves at a rate proportional to the corrosion rate of Zircaloy in water and the surface area of the Zircaloy in contact with water. During corrosion, the Zircaloy cladding degradation rate is determined by Equation (A-8).

$$C_{Zr} = k_{Zr} A_{Zr} \rho_{Zr} \tag{A-8}$$

where,

C_{Zr}	is the Zircaloy cladding degradation rate at time t [kg_{Zr}/a];
k_{Zr}	is the corrosion rate of ZrO_2 in water [m/a];
A_{zr}	is the area of the zircaloy exposed to water [m2]; and
ρ_{Zr}	is the density of Zircaloy [kg/m^3].

The congruent dissolution release rate of contaminant j from the Zircaloy cladding in the failed container at time *t* is given by Equation (A-9).

$$F_{CD,Zr}^{j}(t) = \frac{\left(1 - f_{IRF,Zr}^{j}\right) I_{Zr}^{j}(t) C_{Zr}}{I_{0,Zr} N_{Symmetry}} (t \geq t_F)(t \leq t_{Zr} + t_F) \tag{A-9}$$

where,

$F_{CD,Zr}^{j}(t)$	is the Zircaloy congruent release rate of contaminant j entering the water filled void in the container [mol/a]
$f_{IRF,Zr}^{j}$	is the fraction of contaminant j release instantly from the Zircaloy upon contact with water [-];
$I_{Zr}^{j}(t)$	is the inventory of contaminant j at time t in the Zircaloy cladding [mol];
C_{Zr}	is the Zircaloy cladding degradation rate at time t [kg_{Zr}/a];
$N_{Symmetry}$	is the scaling from a fractional container to a whole container. For a single quarter section of a container $N_{Symetry}$ is 4.
$I_{0,Zr}$	is the initial mass of Zr in a container [kg_{Zr}];
t_F	is the time of container failure [a] defined by Equation (A-2); and
t_{Zr}	is the time after which all the Zircaloy has corroded [a].

The Zircaloy corrosion rate is linear and thus t_{Zr} can be determined by Equation (A-10).

$$t_{Zr} = \frac{I_{0,Zr}}{C_{Zr}} \tag{A-10}$$

A.1.8 Model Source Term

The total source term for a given contaminant is the sum of the instant and congruent release components for the fuel and the Zircaloy cladding and described by Equation (A-11).

$$F_{Total}^{j}(t) = F_{IRF,UO2}^{j}(t) + F_{CD,UO2}^{j}(t) + F_{IRF,Zr}^{j}(t) + F_{CD,Zr}^{j}(t) \tag{A-11}$$

where,

$F_{Total}^{j}(t)$	is the total source term for contaminants j [mol//a];
$F_{IRF,UO2}^{j}(t)$	is the UO_2 instant release component defined in Equation (A-1) [mol/a];

$F^j_{CD,UO2}(t)$	is the UO_2 congruent release component defined in Equation (A-5) [mol/a];
$F^j_{IRF,Zr}(t)$	is the Zircaloy instant release component defined in Equation (A-7) [mol/a]; and
$F^j_{CD,Zr}(t)$	is the Zircaloy congruent release component defined in Equation (A-9) [mol/a].

The release of a given contaminant into the container is defined as a volumetric flux $F^j_{Source}(t)$, proportional to the volume over which the flux is applied and is specified in mol/m^3/a. This flux, defined by Equation (A-12), is applied to the volume representing the container shell.

$$F^j_{Source}(t) = \frac{F^j_{Total}(t)}{V_{cont}} \tag{A-12}$$

where,

V_{cont}	is the water filled volume in the container (see Figure A-5) over which the flux source term is applied [m^3].

Solubility limited contaminants are treated as a special case and modelled using a concentration boundary applied to the interior boundary of the container (see Figure A-5) and is described in Section A.1.9.

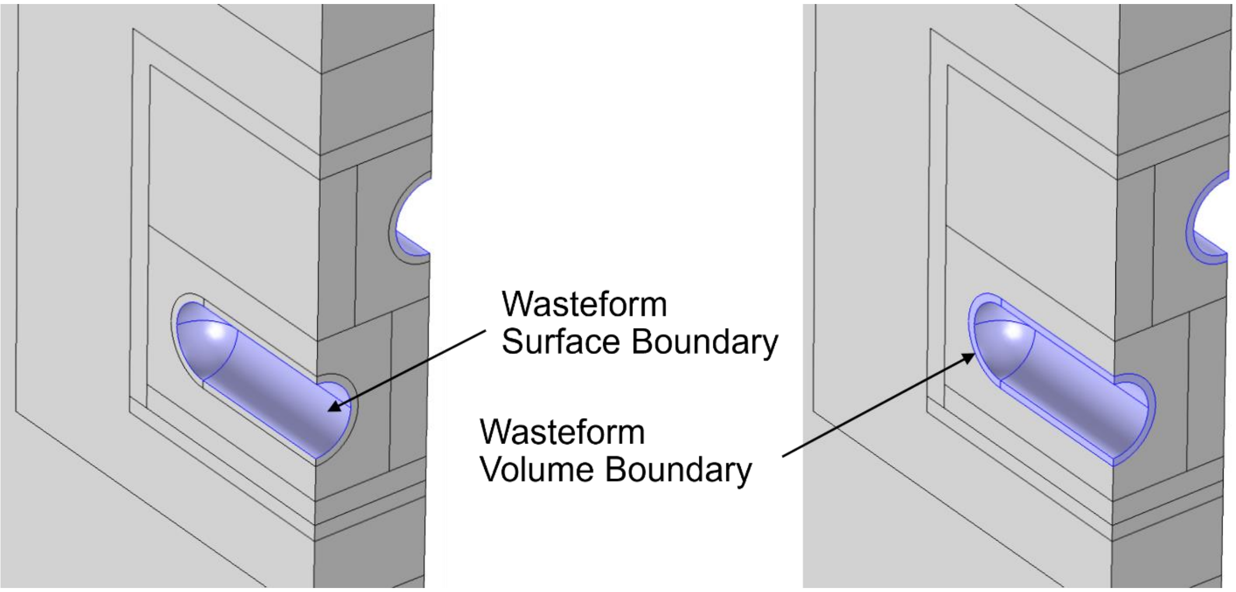


Figure A-5: Wasteform Source Boundary and Volume

A.1.9 Solubility Limited Source Terms

The solubility of a contaminant is a property of the underlying chemical element. For example, both U-234 and U-238 contribute to the same solubility of uranium. The solubility limits for various elements are input as a concentration beyond which an element can precipitate into an immobile solid.

Typically, elements that are solubility limited (e.g., U) have solubility limits that are very low relative to the concentration in the container that could be maintained by the fuel source term defined by Equation (A-12). If solubility limits are considered, the amount of precipitate in the container can be very high. Once the fuel source term is depleted, the precipitate will begin to dissolve and can continue to maintain the solubility limit of an element in the container. Solubility limits can be maintained long after the time after which the fuel has dissolved.

In the ISM-NF, the concentration of each element (sum of all isotopes) in the volume representing the container shell is tracked during model runtime to determine if an element exceeds the user defined solubility limit. If the solubility limit is exceeded, a series of Boolean operators are used to alter model source terms and boundary conditions such that the solubility limit is maintained. In essence, the volumetric flux source is deactivated, and a concentration boundary condition is activated.

This is accomplished using the COMSOL Events Interface. Events in COMSOL are a series of conditions that, once reached, will pause the model solver, re-initialize the model and continue solving. This feature is used to maintain numerical stability when there are discrete changes in model conditions such as a solubility limit being reached.

Initially, the model uses a volumetric flux source as described by Equation (A-12). However, once the solubility limit of a given element is reached, the flux condition is set to zero and a concentration boundary condition is applied to the interior boundary of the container as described in Equation (A-13) and Equation (A-14).

$$\text{if } C^k_{cont}(t) < C^k_{sol} - f_{tol}C^k_{sol} \; then \; F^j_{Source}(t) = \frac{F^j_{Total}(t)}{V_{cont}} \tag{A-13}$$

$$\text{if } C^k_{cont}(t) > C^k_{sol} + f_{tol}C^k_{sol} \; then \begin{cases} F^j_{Source}(t) = 0 \\ C^j_{Boundary}(t) = C^k_{sol}A^j_{iso}(t) \end{cases} \tag{A-14}$$

where,

$C^k_{cont}(t)$	is the volume averaged concentration of element k [mol/m^3] as described by Equation (3-14);
C^k_{sol}	is the solubility limit of element k [mol/m^3];
f_{tol}	is the tolerance in which the solubility limit is maintained [-]. A tolerance is used to prevent frequent changes between the two boundary sets of boundary and source conditions.
$F^j_{Source}(t)$	is the volumetric source term for contaminant j (isotope of element k). If the concentration of element k in the container is below the solubility limit of element k, $F^j_{Source}(t)$ is described by Equation (3-11) and the volumetric flux is applied to the volume shown in Figure A-5. If the concentration of element k in the container exceeds the solubility limit of element k, $F^j_{Source}(t)$ is set to zero;
$C^j_{Boundary}(t)$	is the boundary condition for contaminant j (isotopes of element k). If the concentration of element k is below the solubility limit of element k a no flow boundary condition is applied to the boundary shown in Figure A-5. If the concentration of element k is above the solubility limit of element k, a time varying concentration boundary is used; and
$A^j_{iso}(t)$	is the time-dependent isotopic abundance of contaminant j as described by Equation (3-15).

$$C^k_{cont}(t) = \sum_j^k \frac{\iiint C^j_{cont}(t).dV}{V_{cont}} \tag{A-15}$$

where,

$\iiint C^j_{cont}(t)$	is the integrated amount of contaminant j (isotope of element k) [mol] in the volume shown in Figure A-5; and
V_{cont}	is the water filled volume in the container (see Figure A-5) over which the flux source term is applied [m^3].

$$A^j_{iso}(t) = \frac{I_i(t)}{\sum_i^j I_i(t)} \tag{A-16}$$

where,

$I_j(t)$	is the amount of contaminant j in the fuel at time t [mol]; and
$\sum_j^k I_j(t)$	is the sum of the inventories of all isotopes of element k in the fuel at time t [mol].

Similar to the fuel and the zircaloy congruent release models, the solubility limited release model also tracks how much of a given contaminant has entered the system to determine when the inventory of a given contaminant has been depleted. It is plausible that solubility limited contaminants will take some time to reach the solubility limit or may be only solubility limited for a brief period of time. Therefore, the combined contribution of the volumetric flux and the flux at the concentration boundary are considered when calculated the amount of a given contaminant entering the system. A contaminant is considered depleted if the total mass entering the system exceeds its initial inventory in the fuel. This is equivalent to tracking the amount of a precipitate and modelling the redissolution of the precipitate once the initial source is depleted. Equation (3-16) describes the conditions used to track when the inventory of a solubility limited contaminants is depleted.

$$\begin{gathered} If \int_{t_F}^{t} \iint F^j_{Boundary}(t).dS + \int_{t_F}^{t} \iiint F^j_{Source}(t).dV > I^j_{UO2+Zr}(t) \\ then \begin{cases} F^j_{Source}(t) = 0 \\ C^j_{Boundary}(t) = no\ flux \end{cases} \end{gathered} \tag{A-17}$$

where,

$\int_{t_F}^{t} \iint F^j_{Boundary}(t).dS$	is the time and surface integral of the flux for contaminant j [mol]. The flux is integrated over the fuel source boundary where the concentration boundary is applied (see Figure A-5) and over the time after the container is assumed failed (t_F).
$\int_{t_F}^{t} \iiint F^j_{Source}(t).dV$	is the time and volume integral of the flux for contaminant j [mol]. The flux is integrated over the volume over which the volumetric source term is applied (see Figure A-5) and over the time after the container is assumed failed (t_F).
$I^j_{UO2+Zr}(t)$	is the total initial inventory of contaminant j in the container (in mol) at time t.

A.2 Placement Room

The placement room portion of the near-field model includes the container (Section A.2.1), the engineered barrier system (Section A.2.2), and excavation damaged zone and host rock (Section A.2.3). The primary processes modelled in the placement room portion of the near-field model are the failure of the container (Section A.2.4) and transport through the placement room components (Section A.2.5).

A.2.1 Container

The reference container in the repository is designed to hold 48 used CANDU fuel bundles (Naserifard et al. 2021). The reference container concept has a corrosion-resistant copper coating and a structural steel inner vessel (Figure A-6).

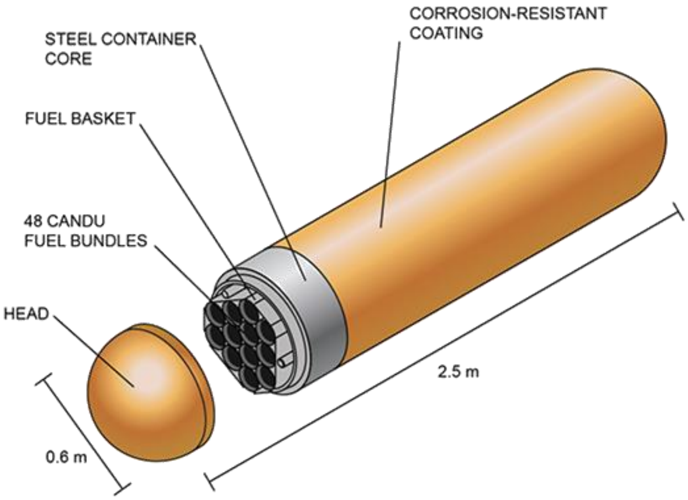


Figure A-6: Container Design

Containers are designed to be robust and durable and intended to withstand the repository conditions essentially indefinitely. However, the post-closure safety assessment model considers the possibility that some containers may fail. The nearfield model assumes that once a container has failed there is sufficient water available to fill the container and to provide a pathway connecting the fuel to the bentonite surrounding the container.

A.2.2 Engineered Sealing Materials

The engineered sealing materials include highly compacted bentonite (HCB) buffer boxes, spacer blocks and bentonite pellets used as gap fill (Naserifard et al. 2021). HCB will be machined to hold and completely surround each used fuel container and is referred to as the buffer box (see Figure A-7). Buffer boxes in the placement rooms will be spaced out with additional HCB spacer blocks. Gaps between the HCB and the walls of the placement room will be filled with bentonite gap fill. The bentonite gap fill will swell when saturated with water and seal the gap. It is expected that the gap fill and HCB will homogenize and remove the distinct boundaries between the materials.

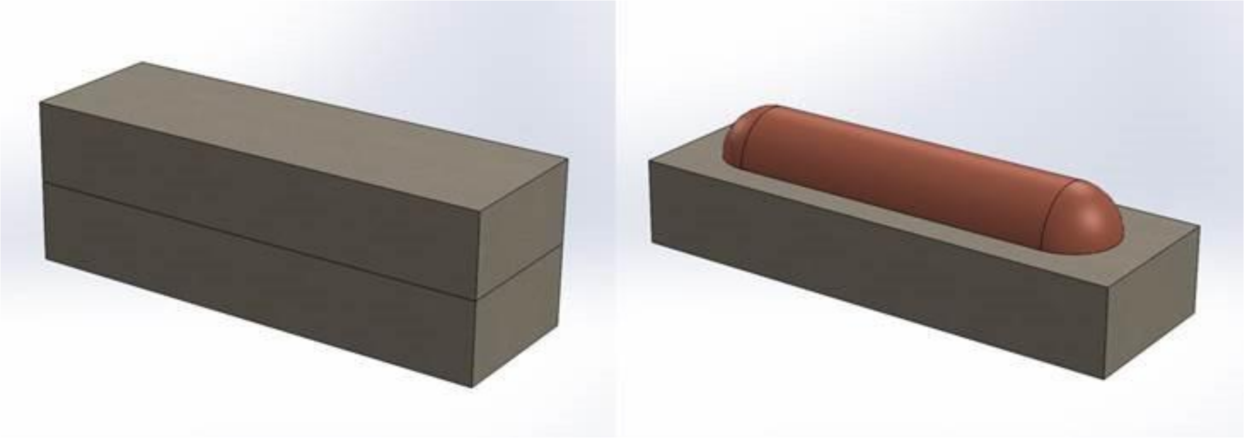


Figure A-7: HCB Buffer Box

A.2.3 Excavation Damaged Zone and Host Rock

Surrounding the placement room is the host rock. Due to the excavation method (e.g. drill and blast) and from rock relaxation into the open excavations, an excavation damaged zone (EDZ) is expected to be present in the rock around placement rooms. Rock in the excavation damaged zone is expected to have higher transport properties than those in the intact host rock. The near-field model includes two distinct zones of excavation damaged outside the placement room. The inner zone is used to represent a region of more permeable EDZ while the outer zone is used to represent a less permeable EDZ zone.

A.2.4 Container Failure

The container model does not model the mechanism of container failure (e.g., corrosion). Instead, the model assumes the container fails at a defined failure time specified in the model input data. Each container is assumed to have two failure zones, the hemi-head and the cylindric container body. With two quarter containers represented in the model there are a total of four possible failure zones. Each of the failure zones can fail at unique times or occur simultaneously. Failure of a container zone is modelled by activating or deactivating source terms using Boolean operators. Section A.1.1 describes how model source terms are controlled and applied in the near-field model.

A.2.5 Transport in the Placement Room

Once the container has failed, water accesses the fuel and contaminants are able to migrate into the engineered barrier system, through the excavation damaged zone and into the intact rock. All materials in the placement room are modelled as saturated porous media. Each unique material in the model (e.g., HCB, inner EDZ) has different material properties and all material properties (e.g., porosity, density) are homogeneous and constant. Transport of contaminants within these materials are governed by the same advection-diffusion process described by Equation (A-18) which is based on Equation 6-2 from COMSOL (2022).

The near-field model solves for the concentration of a contaminants at each node in the model as a function of time and space.

$$\left(\theta_m + \rho_m kd_m^j\right)\frac{\delta C_L^j}{\delta t} + \nabla\left(C_L^j \cdot u_m\right) = \nabla\left(T_s(t) D_{eff,m}^j \nabla C_L^j\right) + R_{decay}^i \qquad \text{(A-18)}$$

where,

θ_m	is the porosity of material m [-];
ρ_m	is the density of material m [kg/m^3]; ρ
kd_m^j	is the linear equilibrium sorption coefficient for contaminants j in material m [m^3/kg].
C_L^j	is the liquid-phase (solute) concentration of contaminants j [mol/m^3];
u_m	is the groundwater velocity vector (with x,y,z components) in material m [m/a];
$D_{eff,m}^j$	is the effective diffusion coefficient of contaminant j in material m [m^2/a];
$T_s(t)$	is the diffusion temperature scaling factor [-] described by Equation (A-19); and
R_{decay}^i	is the reaction term representing loss or creation of radionuclide i (note j=i for radionuclides) from radioactive decay and ingrowth as described in Equation (A-20).

The diffusion temperature scaling factor is determined by taking the ratio of the Stokes-Einstein equation for diffusion coefficients at two temperatures (Einstein, 1905) and is given by:

$$T_s(t) = \frac{T(t) \cdot \mu_0}{T_0 \cdot A \cdot e^{\frac{B}{T(t)}}} \qquad \text{(A-19)}$$

where,

$T_s(t)$	is the diffusion temperature scaling factor [-];
$T(t)$	is the near-field time-dependent temperature [K];
μ_0	is the water viscosity at 293.15K [Pa·s];
T_0	is the initial temperature assumed to be 293.15 [K];
A	is a constant with a value of 2.1x10^{-6} [Pa·s]; and
B	is a constant with a value 1808.5 [K].

Radionuclide decay and ingrowth is represented as a set of reaction terms. One reaction term represents the loss due to decay and depends on the concentration of radionuclide i. If a contaminants is a member of a chain, a second reaction represents ingrowth from the parent (contaminants i-1). Both these reaction terms are defined in Equation (A-20) and described in the reactions section of Chapter 6 of COMSOL (2022).

$$R_{decay}^i = \left(\theta_m + \rho_m kd_m^{i-1}\right)\lambda_{i-1} C_L^{i-1}(t) - \left(\theta_m + \rho_m kd_m^i\right)\lambda_i C_L^i(t) \qquad \text{(A-20)}$$

where,

R_{decay}^i	is the reaction term representing loss or creation of radionuclide i from radioactive decay and ingrowth as described in Equation (A-20).
θ_m	is the porosity of material m [-];
ρ_m	is the density of material m [kg/m^3];
kd_m^i	is the linear equilibrium sorption coefficient for radionuclide i in material m [m^3/kg].
λ_i	is the radionuclide decay constant of radionuclide i [a^{-1}];
C_L^i	is the liquid-phase (solute) concentration of radionuclide i [mol/m^3];

A.3 Model Boundary Conditions

There are three main boundary conditions applied in the near-field model.

- The source term boundary conditions described in Section A.1.8 and Section A.1.9;
- A zero-concentration boundary condition applied to the external model boundary (see Figure A-8a); and
- A no flux or symmetry boundary condition applied along the sides of the model (see Figure A-8b).

Boundary conditions were selected to both optimize model performance (e.g., reduce the extent of the model domain) and be conservative.

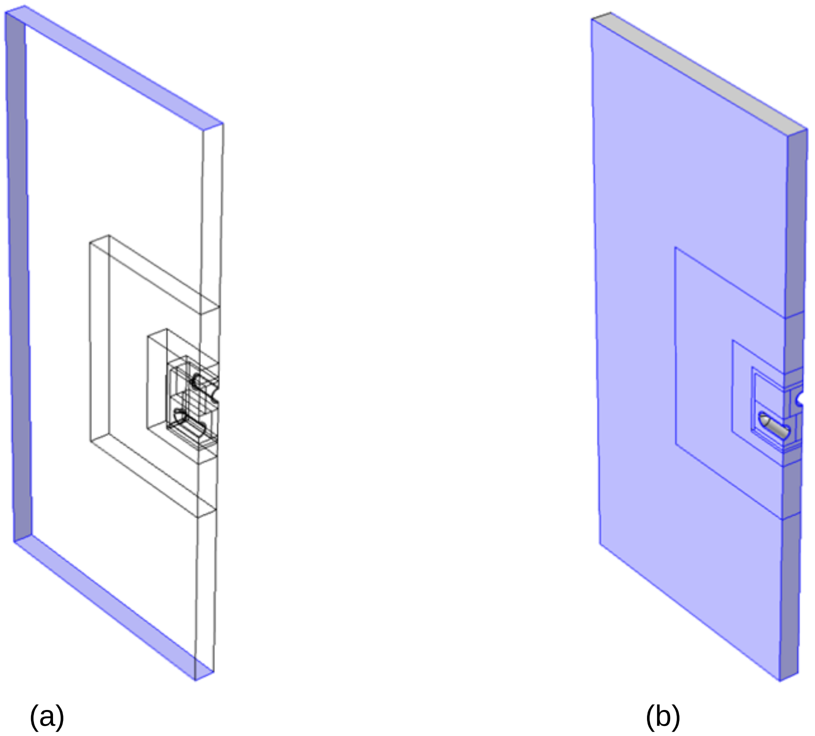

(a) (b)

Figure A-8: (a) Zero Concentration Boundary Condition, (b) Symmetry Boundary Condition

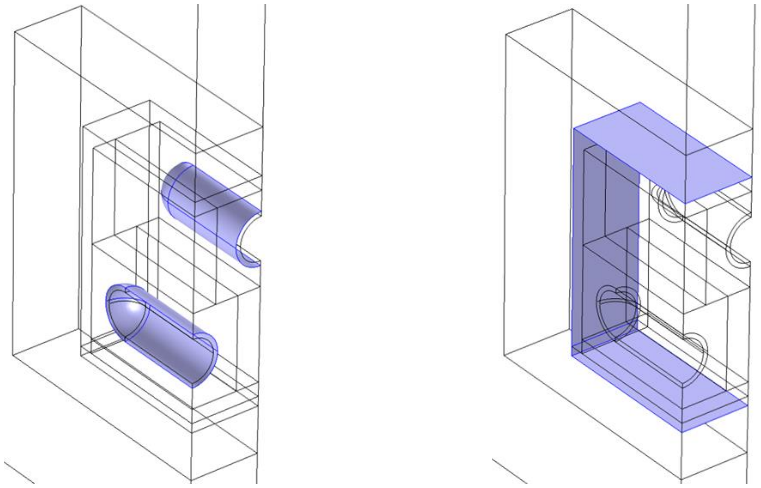
A limitation of the no-flux or symmetry boundary condition applied along the sides of the model is that transport along the placement room (e.g., along the EDZ or concrete floor) is not represented. In practice, if transport along the placement room is expected to be a significant component of the near-field transport, an interface close to the container (e.g., (a) in Figure A-9) is used and transport along the room is represented in the ISM-GEO model which can accurately calculate groundwater flow fields and transport along the placement rooms.

A.4 Interface with the Geosphere Model

The near-field model includes 4 interfaces over which output to the geosphere is calculated, namely:

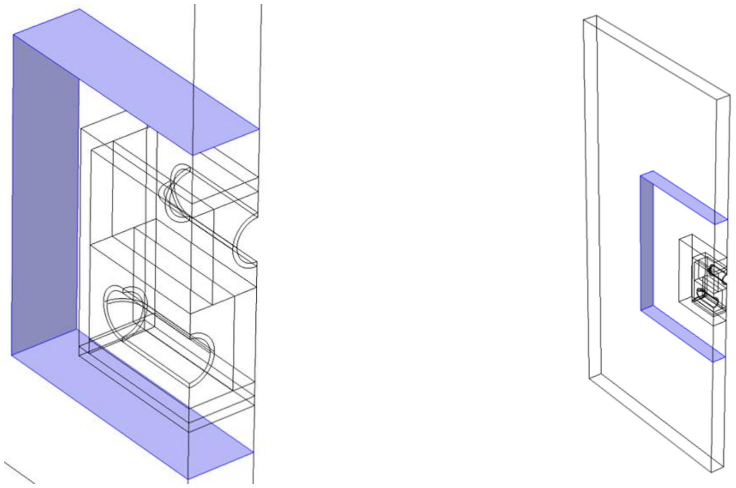
- the container / HCB interface;
- the HCB / inner EDZ interface;
- the inner EDZ / outer EDZ interface; and
- the outer EDZ / intact rock interface.

Each interface is highlighted in blue in Figure A-9. The output from the near-field model is the surface integrated flux (i.e., total release rate) for each contaminants crossing the bentonite EDZ interfaces shown in Figure A-9.



a) Container / HCB Interface

b) HCB / Inner EDZ Interface



c) Inner EDZ / Outer EDZ Interface

d) Outer EDZ / Intact Rock Interface

Figure A-9: Near-field – Geosphere Model Interfaces

The total release of a contaminants from the near-field represents either the net release rate from one or two quarter sections of a failed container. The total release rate of a contaminants from the near-field model is linearly scaled to represent the rate of a contaminants entering the geosphere for any number of failed containers as described by Equation (3-19).

$$X_{GEO}^{j}(t) = X_{NF}^{j}(t) N_{symmetry} N_{Cont} f_{units}^{j} f_{time} \qquad \text{(A-21)}$$

where,

$X_{GEO}^{j}(t)$	is the total release rate of contaminants j entering the geosphere [kg/s];
$X_{NF}^{j}(t)$	is the near-field release rate of contaminants j through the bentonite-EDZ interface (boundary highlighted in blue in Figure A-9) for one or two failed quarter containers [mol/a]. This is defined as the surface integral of the flux [mol/m^2/a] through the bentonite-EDZ boundary and is defined by Equation (3-17);
$N_{Symmetry}$	is the scaling from a fractional container to a whole container [-];
N_{Cont}	is the number of failed containers in the repository [-];
f_{units}^{j}	is the conversion factor used to convert from mol to kg or Bq for contaminants j [kg/mol or Bq/mol]. The outputs are typically converted to kg/s or Bq/a; and
f_{time}	is the conversion factor used to convert the time units to the desired output unit (e.g., from years to seconds [s/a]).

$$X_{NF}^{j}(t) = \iint \Phi_{NF}^{j}(t).\,dS \qquad \text{(A-22)}$$

where,

$\boldsymbol{\Phi_{NF}^{i}(t)}$ is the flux (mol/m^2/a) passing through the various near-field-geosphere interfaces (the boundaries highlighted in blue in Figure A-9).

APPENDIX B – SUMMARY OF ISM THEORY CHANGES

Version	Summary of ISM Theory Changes
1.0	ISM v1.0 consisted of: ISM-NF: • Radioactive decay representing decay and ingrowth of species; • Instant release of some fraction of the fuel and cladding inventory upon failure of the container; • Congruent release of remaining inventory as the fuel matrix and cladding degrades; • Solubility limited release of species that exceed defined solubility limits in the container; and • Transport via diffusion and advection (with sorption) of dissolved species out of the container and through the engineered barrier system and the excavation damaged zone. ISM-GEO: • Radioactive decay representing decay and ingrowth of species; • Flow and transport within the subsurface (surface flow and transport are not considered); • Materials are assumed to be saturated porous media; • Fractures or other geosphere features are represented using an effective porous media approach; and • A domestic well. ISM-BIO: • Radioactive decay representing decay and ingrowth of species; • Soil model that estimates concentration in subsoil and surface soils for up to two fields (garden and forage); • Soil model processes include terrestrial discharge from the geosphere, irrigation, leaching, erosion, cropping and volatilization; • Surface water model that estimates concentration in surface waters for up to three unique surface water features such as lakes, rivers, and wetlands; • Surface water model processes include aquatic discharge from the geosphere, flow between surface water features, flow from the soil model, volatilization and sedimentation; • Equilibrium atmosphere model that estimates air concentration of species above the most contaminated field; • Equilibrium sediment model that estimates the sediment concentration in each surface water body; • Well and domestic water use model that estimates concentration of species in well water, groundwater, domestic use water and irrigation water; • Comparison of environmental media concentrations (soils, surface waters, groundwater, air and sediments) with acceptance criteria for chemically hazardous species. • Calculation of radionuclide concentrations in plants and animals based on concentration in environmental media concentrations described above; and

	• Calculation of radiological doses to a critical group for two unique lifestyles (self-sufficient farm and hunter-gatherer) and three age groups (adult, child and infant).
1.01	ISM v1.0.1 included the following theory changes: ISM-NF: • Changed rock and excavation damaged zone tortuosity to be species dependent.
1.1	ISM v1.1 included the following theory changes: ISM-NF: • Added time-dependent temperature dependence to diffusion coefficients; • Added precipitation / redissolution model for solubility limited species; and • Replaced boundary source term with a volumetric source term. ISM-GEO-RV (Revell Site) and ISM-GEO-SB (South Bruce Site): • Developed initial Revell and South Bruce Site geosphere models; • Added a discrete fracture network representation fractures and faults using a dual-continuum approach and model theory; and • Added new (municipal and single family) wells ISM-BIO-RV / ISM-BIO-SB: • Developed Revell and South Bruce Site specific biosphere models; • Added specific-activity models for I-129 and C-14; • Added an indoor air model and revised the outdoor air model; • Added new site-specific lifestyles for the Revell and South Bruce Sites; • Added new site-specific surface waterbodies (e.g., Teeswater river and Greenock swamp for South Bruce and Lakes A, B, and C for Revell); and • Added new (municipal and single family) wells for Revell and South Bruce.
1.2	ISM v1.2 included the following theory changes: ISM-NF: • Replaced free water diffusion coefficients with effective diffusion coefficients. ISM-GEO-RV and ISM-GEO-SB • Several model changes were made to increase site specific nature of the geosphere models; however the model theory did not fundamentally change. ISM-BIO-RV and ISM-BIO-SB • Updated terrestrial discharge from the geosphere to consider if a field is irrigated; • Updated the fraction of time spent outdoors to be age specific; • Updated the domestic water use to depend to depend on lifestyle; and • Added additional site-specific waterbodies (e.g., Teeswater river and Greenock swamp were subdivided into multiple upstream and downstream components).

1.3	ISM v1.3 included the following theory changes: ISM-NF • Updated numerical solver settings to improve numerical stability • Added a fractional fuel dissolution model ISM-GEO-RV and ISM-GEO-SB • Updated the representation of the Revell and South Bruce geospheres at four distinct domains and resolutions: Revell model domains consist of: (1) Regional Scale – regional scale domain used to determine model boundary conditions (2) Site Scale – a domain capturing the repository site (3) Panel Scale – sub-domain(s) at the scale of a single panel of the repository (4) Room Scale – sub-domain(s) at the scale of a few placement rooms. South Bruce model domains consist of: (1) Regional Scale – regional scale domain used to determine model boundary conditions (2) Medium Scale – an extended model domain larger than the Site Scale intended to capture more distant discharge / transport from the repository (3) Site Scale – a domain capturing the repository site (4) Room Scale – sub-domain(s) at the scale of a few placement rooms. • Updated ISM-GEO to be consistent with 2023 Engineering and Geoscience data clearances • Updated discharge areas in ISM-GEO models to reflect the latest model domain changes (bullet one above) and the new biosphere surface water features (ISM-BIO changes below) ISM-BIO • Added the indigenous and town resident lifestyles • Updated the main surface waterbody to be dynamically calculated (as maximally contaminated) instead of user defined • Added additional surface water bodies and wetlands to the ISM-BIO models
1.4	<u>ISM</u> • Retired versions of the ISM models representing the South Bruce Site following the site selection decision and removed South Bruce related content from the ISM theory manual. No changes were made to the ISM-GEO and ISM-BIO models representing the Revell Site. <u>ISM-NF</u>

	• ISM-NF becomes an optional component of ISM v1.4 (model overview and theory moved to Appendix A). ISM-WF Development of a new wasteform model (ISM-WF). The ISM-WF model is used to estimate radionuclide and element “source terms” from a variety of wasteforms that may be disposed of in the DGR (e.g., CANDU fuels, prototype fuels, research fuels, and low level wastes).