## Document History

<table>
<thead>
<tr>
<th>Title:</th>
<th>ISM v1.0 Theory Manual</th>
</tr>
</thead>
<tbody>
<tr>
<td>Revision:</td>
<td>R000</td>
</tr>
<tr>
<td>Date:</td>
<td>December 2019</td>
</tr>
</tbody>
</table>

Nuclear Waste Management Organization

<table>
<thead>
<tr>
<th>Authored by:</th>
<th>M. Gobien and C. Medri</th>
</tr>
</thead>
<tbody>
<tr>
<td>Verified by:</td>
<td>A. Boyer, S. Briggs, and J. Chen</td>
</tr>
<tr>
<td>Reviewed by:</td>
<td>M. Ion, P. Gierszewski</td>
</tr>
<tr>
<td>Approved by:</td>
<td>D. Wilson</td>
</tr>
</tbody>
</table>

## Revision Summary

<table>
<thead>
<tr>
<th>Revision Number</th>
<th>Date</th>
<th>Description of Changes/Improvements</th>
</tr>
</thead>
<tbody>
<tr>
<td>R000</td>
<td>2019-12</td>
<td>Initial issue</td>
</tr>
</tbody>
</table>
ABSTRACT

Title: ISM v1.0 Theory Manual
Report No.: NWMO-TR-2019-06
Author(s): M. Gobien and C. Medri
Company: Nuclear Waste Management Organization
Date: December 2019

Abstract

This report describes the theory for the Integrated System Model (ISM) v1.0. The ISM is intended to assess postclosure safety of a deep geologic repository for used CANDU fuel. The system model is composed of a series of linked models representing the near field, the geosphere and the biosphere.

The near field model (ISM-NF) consists of the waste form, containers, engineered barrier system, and excavation damaged zone surrounding the placement room. The near field model includes the failure of some containers, degradation of the used fuel, and transport of species from the failed containers and through the engineered barrier system and excavation damaged zones. The near field model interfaces with the geosphere model by passing fluxes of species entering the excavation damaged zone from the engineered barrier system.

The geosphere model (ISM-GEO) describes the movement of species from the repository via the groundwater in the rock mass and fractures to the surface environment. The source term in the geosphere model is determined by the near field model. The interface with the biosphere model is fluxes of species to a domestic water well, as well as to aquatic and terrestrial discharge areas at surface.

The biosphere model (ISM-BIO) describes the movement of species between surface water, soils, atmosphere, vegetation, animals and humans. The biosphere model estimates concentrations of species in environmental media (soil, sediment, groundwater, surface water and air). Based on the environmental media concentrations, the model estimates the radiological dose to a critical group living near the repository.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>ABSTRACT</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Background</td>
<td>1</td>
</tr>
<tr>
<td>1.2 Scope</td>
<td>2</td>
</tr>
<tr>
<td>2. RADIOACTIVE DECAY AND INGROWTH</td>
<td>2</td>
</tr>
<tr>
<td>3. ISM-NF MODEL</td>
<td>3</td>
</tr>
<tr>
<td>3.1 ISM-NF Model Overview</td>
<td>4</td>
</tr>
<tr>
<td>3.2 Wasteform</td>
<td>5</td>
</tr>
<tr>
<td>3.2.1 Instant Release from UO₂ Matrix</td>
<td>6</td>
</tr>
<tr>
<td>3.2.2 Congruent Release from the Fuel Matrix</td>
<td>7</td>
</tr>
<tr>
<td>3.2.3 Instant Release from the Zircaloy Cladding</td>
<td>9</td>
</tr>
<tr>
<td>3.2.4 Congruent Release from Zircaloy Cladding</td>
<td>10</td>
</tr>
<tr>
<td>3.2.5 Model Source Term</td>
<td>11</td>
</tr>
<tr>
<td>3.2.6 Solubility Limits, Precipitation, and Dissolution</td>
<td>12</td>
</tr>
<tr>
<td>3.3 Placement Room</td>
<td>13</td>
</tr>
<tr>
<td>3.3.1 Container</td>
<td>13</td>
</tr>
<tr>
<td>3.3.2 Engineered Barrier System</td>
<td>13</td>
</tr>
<tr>
<td>3.3.3 Excavation Damaged Zone</td>
<td>14</td>
</tr>
<tr>
<td>3.3.4 Container Failure</td>
<td>14</td>
</tr>
<tr>
<td>3.3.5 Transport in the Placement Room</td>
<td>15</td>
</tr>
<tr>
<td>3.4 Model Boundary Conditions</td>
<td>16</td>
</tr>
<tr>
<td>3.5 Interface with the Geosphere Model</td>
<td>17</td>
</tr>
<tr>
<td>4. ISM-GEO MODEL</td>
<td>19</td>
</tr>
<tr>
<td>4.1 Geosphere Model Overview</td>
<td>19</td>
</tr>
<tr>
<td>4.2 Geosphere-Near Field Interface</td>
<td>21</td>
</tr>
<tr>
<td>4.3 Geosphere Model Theory</td>
<td>21</td>
</tr>
<tr>
<td>4.3.1 Subsurface Flow</td>
<td>22</td>
</tr>
<tr>
<td>4.3.2 Subsurface Flow in Fractures and Aquifers</td>
<td>23</td>
</tr>
<tr>
<td>4.3.3 Subsurface Flow in the Well</td>
<td>23</td>
</tr>
<tr>
<td>4.3.4 Transport in Saturated Porous Media</td>
<td>24</td>
</tr>
<tr>
<td>4.3.5 Transport in the Well</td>
<td>25</td>
</tr>
<tr>
<td>4.3.6 Boundary Conditions</td>
<td>26</td>
</tr>
<tr>
<td>4.3.6.1 Flow Boundary Conditions</td>
<td>26</td>
</tr>
<tr>
<td>4.3.6.2 Transport Boundary Conditions</td>
<td>26</td>
</tr>
<tr>
<td>4.3.6.3 ISM-GEO Boundary Conditions</td>
<td>26</td>
</tr>
<tr>
<td>4.4 Interface with the Biosphere Model</td>
<td>27</td>
</tr>
<tr>
<td>5. ISM-BIO MODEL</td>
<td>29</td>
</tr>
<tr>
<td>5.1 Biosphere Model Overview</td>
<td>29</td>
</tr>
<tr>
<td>5.2 Interface with Geosphere Model</td>
<td>32</td>
</tr>
<tr>
<td>5.3 Soil Concentration</td>
<td>33</td>
</tr>
<tr>
<td>5.3.1 Overview</td>
<td>33</td>
</tr>
<tr>
<td>5.3.2 Garden Field</td>
<td>34</td>
</tr>
<tr>
<td>5.3.2.1 Self-Sufficient Farmer Lifestyle</td>
<td>34</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>5.3.2.2</td>
<td>Hunter-Gatherer Lifestyle</td>
</tr>
<tr>
<td>5.3.3</td>
<td>Forage Field</td>
</tr>
<tr>
<td>5.3.3.1</td>
<td>Self-Sufficient Farmer Lifestyle</td>
</tr>
<tr>
<td>5.3.3.2</td>
<td>Hunter-Gatherer Lifestyle</td>
</tr>
<tr>
<td>5.3.4</td>
<td>Sub-Soil</td>
</tr>
<tr>
<td>5.3.5</td>
<td>Surface Soil</td>
</tr>
<tr>
<td>5.3.5.1</td>
<td>Irrigation from Well Water</td>
</tr>
<tr>
<td>5.3.5.2</td>
<td>Irrigation from Surface Water</td>
</tr>
<tr>
<td>5.3.5.3</td>
<td>Leaching</td>
</tr>
<tr>
<td>5.3.5.4</td>
<td>Erosion</td>
</tr>
<tr>
<td>5.3.5.5</td>
<td>Cropping</td>
</tr>
<tr>
<td>5.3.5.6</td>
<td>Volatilization</td>
</tr>
<tr>
<td>5.3.5.7</td>
<td>Surface Soil Concentration</td>
</tr>
<tr>
<td>5.4</td>
<td><strong>Surface Water Concentration</strong></td>
</tr>
<tr>
<td>5.4.1</td>
<td>Surface Water Sources</td>
</tr>
<tr>
<td>5.4.1.1</td>
<td>Aquatic Discharge</td>
</tr>
<tr>
<td>5.4.1.2</td>
<td>Flow between Surface Water Features</td>
</tr>
<tr>
<td>5.4.1.3</td>
<td>Flow from Surface Soil</td>
</tr>
<tr>
<td>5.4.1.4</td>
<td>Discharge of Domestic Water</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Surface Water Losses</td>
</tr>
<tr>
<td>5.4.2.1</td>
<td>Flow between Surface Water Features</td>
</tr>
<tr>
<td>5.4.2.2</td>
<td>Volatilization</td>
</tr>
<tr>
<td>5.4.2.3</td>
<td>Sedimentation</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Surface Water Concentration</td>
</tr>
<tr>
<td>5.5</td>
<td><strong>Well Water Concentration</strong></td>
</tr>
<tr>
<td>5.6</td>
<td>Groundwater Concentration</td>
</tr>
<tr>
<td>5.7</td>
<td>Domestic Water Concentration</td>
</tr>
<tr>
<td>5.8</td>
<td><strong>Irrigation Water Concentration</strong></td>
</tr>
<tr>
<td>5.9</td>
<td>Sediment Concentration</td>
</tr>
<tr>
<td>5.10</td>
<td>Atmosphere Concentration</td>
</tr>
<tr>
<td>5.11</td>
<td>Concentration in Plants and Animals</td>
</tr>
<tr>
<td>5.11.1</td>
<td>Plants</td>
</tr>
<tr>
<td>5.11.2</td>
<td>Animals</td>
</tr>
<tr>
<td>5.11.2.1</td>
<td>Livestock</td>
</tr>
<tr>
<td>5.11.2.2</td>
<td>Aquatic Biota</td>
</tr>
<tr>
<td>5.11.2.3</td>
<td>Wildlife</td>
</tr>
<tr>
<td>5.12</td>
<td><strong>Human Dose Pathways</strong></td>
</tr>
<tr>
<td>5.12.1</td>
<td>Ingestion Dose Rates</td>
</tr>
<tr>
<td>5.12.1.1</td>
<td>Food</td>
</tr>
<tr>
<td>5.12.1.2</td>
<td>Water</td>
</tr>
<tr>
<td>5.12.1.3</td>
<td>Soil</td>
</tr>
<tr>
<td>5.12.1.4</td>
<td>Sediment</td>
</tr>
<tr>
<td>5.12.2</td>
<td>Inhalation Dose Rates</td>
</tr>
<tr>
<td>5.12.3</td>
<td>External Dose Rates</td>
</tr>
<tr>
<td>5.12.3.1</td>
<td>Air Immersion Rates</td>
</tr>
<tr>
<td>5.12.3.2</td>
<td>Water Immersion Dose Rates</td>
</tr>
<tr>
<td>5.12.3.3</td>
<td>Groundshine Dose Rates</td>
</tr>
<tr>
<td>5.12.3.4</td>
<td>Beachshine Dose Rates</td>
</tr>
<tr>
<td>5.12.4</td>
<td>Total Dose Rate</td>
</tr>
<tr>
<td>5.13</td>
<td><strong>Concentration of Non-Radiological Species</strong></td>
</tr>
</tbody>
</table>
6. SUMMARY ......................................................................................................................... 65

REFERENCES .......................................................................................................................... 67

LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-1</td>
<td>Volatilization Rates</td>
<td>41</td>
</tr>
<tr>
<td>5-2</td>
<td>Field Types and Associated Plant Types</td>
<td>51</td>
</tr>
<tr>
<td>5-3</td>
<td>Animal Groupings</td>
<td>54</td>
</tr>
</tbody>
</table>

LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-1</td>
<td>Illustration of the Multi-BARRIER Concept for a Deep Geologic Repository</td>
<td>1</td>
</tr>
<tr>
<td>3-1</td>
<td>ISM-NF Model Geometry</td>
<td>3</td>
</tr>
<tr>
<td>3-2</td>
<td>CANDU Fuel Bundle</td>
<td>5</td>
</tr>
<tr>
<td>3-3</td>
<td>Distribution of various radionuclides within a used fuel element</td>
<td>6</td>
</tr>
<tr>
<td>3-4</td>
<td>Wasteflorm (Source) Boundary</td>
<td>12</td>
</tr>
<tr>
<td>3-5</td>
<td>Container Design</td>
<td>13</td>
</tr>
<tr>
<td>3-6</td>
<td>Buffer Box</td>
<td>14</td>
</tr>
<tr>
<td>3-7</td>
<td>Container Failure Model</td>
<td>15</td>
</tr>
<tr>
<td>3-8</td>
<td>(a) Zero Concentration Boundary Condition, (b) Symmetry Boundary Condition</td>
<td>17</td>
</tr>
<tr>
<td>3-9</td>
<td>Buffer-EDZ Interface</td>
<td>18</td>
</tr>
<tr>
<td>4-1</td>
<td>Example of ISM-GEO Model Geometry</td>
<td>20</td>
</tr>
<tr>
<td>4-2</td>
<td>Geosphere - Near Field Model Interface</td>
<td>21</td>
</tr>
<tr>
<td>4-3</td>
<td>Head Boundaries</td>
<td>27</td>
</tr>
<tr>
<td>4-4</td>
<td>Advective Transport Pathways in Example Model</td>
<td>28</td>
</tr>
<tr>
<td>4-5</td>
<td>Geosphere - Biosphere Model Interface in Example Model Showing Repository</td>
<td>28</td>
</tr>
<tr>
<td></td>
<td>Footprint Projected to Surface and Advective Discharge Points</td>
<td></td>
</tr>
<tr>
<td>5-1</td>
<td>Transfer Model between Biosphere Compartments</td>
<td>30</td>
</tr>
<tr>
<td>5-2</td>
<td>Connection between Model Compartments and Components</td>
<td>30</td>
</tr>
<tr>
<td>5-3</td>
<td>ISM-BIO Dose Pathways</td>
<td>32</td>
</tr>
<tr>
<td>5-4</td>
<td>Illustration of Geosphere-Biosphere Interface</td>
<td>33</td>
</tr>
<tr>
<td>5-5</td>
<td>Soil Transport Processes</td>
<td>34</td>
</tr>
<tr>
<td>5-6</td>
<td>Surface Water Transport Processes</td>
<td>42</td>
</tr>
</tbody>
</table>
1. INTRODUCTION

1.1 Background

This report describes the Integrated System Model (ISM) for assessing postclosure safety of a deep geologic repository for used CANDU fuel. The system model is composed of a series of linked submodels – the nearfield (ISM-NF), the geosphere (ISM-GEO) and the biosphere (ISM-BIO).

The system model was developed to address the configuration of a deep geologic repository for used nuclear fuel with in-room placement of durable containers surrounded by a dense clay engineered barrier system. The repository is located deep underground in stable, saturated rock. An illustrative figure of such a repository is provided in Figure 1-1.

The ISM-NF model describes the waste form, containers, engineered barrier system, and excavation damaged zone surrounding the placement room. It assumes the failure of some containers, degradation of the used fuel by water, and transport of species out of the container and through the engineered barrier system and excavation damaged zone. The ISM-GEO model describes the movement of species from the repository via the groundwater through the rock mass and fractures, to the surface environment. The ISM-BIO model determines the concentration of species in environmental media (e.g., surface water, groundwater, sediments, soils, air) and estimates the consequent radiological dose to a critical group living near the repository.

Figure 1-1: Illustration of the Multi-Banner Concept for a Deep Geologic Repository
1.2 Scope

This report describes the main equations governing in the ISM v1.0 computer code as well as underlying assumptions. References are given where more detailed or background information is published. Recommended values for the parameters are specific to each safety assessment, and are not included here.

In general numerical solution techniques are not discussed in this report. The ISM v1.0 code is built using three commercially available programs, namely COMSOL, HydroGeoSphere (HGS) and AMBER. Numerical solutions for these commercial codes are proprietary though some numerical techniques are discussed in the software documentation, namely Aquanty (2013), COMSOL (2018), and Quintessa (2018).

The report contains four main sections, radioactive decay and ingrowth (Section 2), the ISM-NF model (Section 3), the ISM-GEO model (Section 4), and the ISM-BIO model (Section 5).

Throughout this report variables applicable to species (meaning radionuclides or stable isotopes) are denoted with the subscript or superscript j. Variables only applicable to radionuclides are denoted with subscript or superscript i is used. Variables applicable to elements (meaning the sum of all isotopes of a given element) are denoted with subscript or superscript k.

2. RADIOACTIVE DECAY AND INGROWTH

The most notable and common process included in all components of the ISM v1.0 models is radioactive decay and ingrowth. Decay of a single radionuclide or nuclide i is described by:

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

(2-1)

The solution to this first-order differential equation is:

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

(2-2)

Where,

- $N_i(t)$ is the amount of a radionuclide i at time t;
- $N_{i,0}$ is the initial amount of a given radionuclide;
- $\lambda_i$ is the decay rate of a radionuclide i; and
- t is time

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:

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

(2-3)

In the ISM-NF, ISM-GEO, and ISM-BIO 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. **ISM-NF MODEL**

The ISM-NF model (also referred to as the near field model) consists of the waste form, containers, engineered barrier system, and excavation damaged zone surrounding the placement room and the processes therein. The near field model geometry (Figure 3-1) includes a representation the container interior, the engineered barrier system and excavation damaged zone.

![Figure 3-1: ISM-NF Model Geometry](image)

Several assumptions about the near-field model geometry and boundary conditions have been made in order to simplify or reduce execution time of the model. These include:

- The wasteform (i.e., fuel) geometry is not explicitly modelled in the ISM-NF. Species enter the nearfield model via a flux or constant concentration boundary condition applied across the wasteform (source) boundary highlighted in blue in Figure 3-1.
- The model represents a one quarter section each of two containers. The model is divided along planes of symmetry within the nearfield.
• Model inputs such as the mass of the fuel and fuel surface area are input for a whole container and then scaled down by a symmetry factor $N_{\text{Symmetry}}$ to make inputs appropriate for each quarter scale container model (i.e., $N_{\text{Symmetry}}$ is equal to 4).
• Release rates can be applied to one or both of the two quarter-scale containers in the ISM-NF model.
• Release rate results of the quarter scale ISM-NF model are scaled up by $N_{\text{Symmetry}}$ so that computed results are reflective of whole containers (up to two). Results can be further scaled by $N_{\text{Cont}}$ to represent any number of failed containers.
• Several placement room features, such as the room lookouts, are not explicitly modelled.
• Placement rooms and surrounding excavation damaged zones are assumed to be rectangular but in reality would include some rounding.
• Model assumes a zero concentration boundary at the external model boundary (see Section 3.4).

3.1 ISM-NF Model Overview

The repository concept is designed to isolate and contain radioactive wastes essentially indefinitely. However, the ISM is a postclosure safety assessment model, which considers the consequence of failure of some containers. The 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 ISM-NF model can be divided into the conceptual wasteform model, and the 3D placement room model (container, engineered barrier system and excavation damaged zone) in terms of processes considered. The ISM-NF model includes the following processes:

• Instant release of some fraction of the fuel and Zircaloy inventory upon failure of the container;
• Congruent release of remaining inventory as the UO$_2$ fuel matrix and Zircaloy degrades;
• Solubility limited release of species at the fuel source boundary that exceed defined solubility limits;
• Radioactive decay and ingrowth; 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.

The conceptual nearfield model makes a number of assumptions regarding the processes included in the ISM-NF model. These include:

• The nearfield is assumed to be fully saturated at the time of container failure and all model features are treated as saturated porous media.
• Containers are filled with water upon failure of the container and a gas phase is not considered.
• The effect of the Zircaloy cladding on delaying or inhibiting fuel corrosion is ignored.
• Containers are assumed to retain their general integrity such that the container internal volume is not reduced even when failed.
• The build-up of corrosion products within the container or migration of bentonite into the container is not modelled.
The nearfield model is assumed to be at a constant temperature. Effects of temperature on species transport may be included via the choice of diffusion coefficient.

Advective velocities are not computed by the ISM-NF model. Velocities are input as vectors with magnitude and direction set in the model input. Unique velocities can be applied in the container, engineered barrier system and excavation damaged zone model domains.

A linear equilibrium sorption (Kd) model is assumed in the ISM-NF model. Unique sorption coefficients can be applied in the container, engineered barrier system and excavation damaged zones.

Material properties (ie porosity, density, etc) within container interior, engineered barrier system, and excavation damaged zones are assumed to be homogeneous and constant.

Formation and transport of colloids is not modelled.

The output of the ISM-NF model is time dependent transport (in mol/a) of each species entering the geosphere. Transport to the geosphere is calculated by integrating the flux through the interface between the engineered barrier system and excavation damaged zone. To be clear, while the ISM-NF model calculates transport into a portion of the near-field rock as shown in Figure 3-1, the output flux from the near-field model is integrated over the model internal boundary between engineered barrier and rock. This flux is used as a source term in the ISM-GEO model.

3.2 Wasteform

The reference wasteform is a CANDU used fuel bundle, consisting of irradiated UO₂ encased in Zircaloy cladding (Figure 3-2).

![CANDU Fuel Bundle](image)

Figure 3-2: CANDU Fuel Bundle

The inventory of used fuel in interim storage consists primarily of 28-element and 37-element natural uranium CANDU fuel bundles and their variants (Gobien and Ion, 2019). The fuel
geometry is not represented in detail in the near field model (see Figure 3-1) so the exact fuel type is largely irrelevant. Variations in the fuel type, composition, burnup and power are captured in the inventory. The wasteform model includes releases from the UO$_2$ fuel matrix and the Zircaloy cladding.

The detailed wasteform model theory is described in Section 3.2.1 through 3.2.5. Note that other wasteforms may be analyzed if they can be represented by a wasteform and cladding material, with the appropriate inventory and degradation input parameters.

### 3.2.1 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 3-3 (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 species) 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.

![Figure 3-3: Distribution of various radionuclides within a used fuel element](image-url)
In particular, a rapid release and a slow release process 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 3.2.2.

The rate of release of species $j$ from the UO$_2$ matrix by instant release is given by Equation (3-1). The instant release occurs via a smoothed (numerically stable) rectangular function at the time of container failure.

$$F_{IRF,UO2}^j(t) = \frac{f_{IRF,UO2}^j I_{UO2}^j(t) \delta(t_F, t_{IRF})}{N_{Symmetry}}$$

(3-1)

Where,

- $F_{IRF,UO2}^j(t)$ is the UO$_2$ instant release rate of species $j$ entering the container [mol/a];
- $f_{IRF,UO2}^j$ is the fraction of species $j$ release instantly from the UO$_2$ matrix upon contact with water [ ];
- $I_{UO2}^j$ is the inventory of species $j$ at time $t$ in the UO$_2$ fuel 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 minimum time of container zone failures [a] defined by equation (3-2); 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 $N_{Symmetry}$ is 4.

$$t_F = \min(t_b, t_h)$$

(3-2)

Where,

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

3.2.2 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$_2$ is the redox conditions in the surrounding groundwater (Shoesmith et al. 1997, 2007). Reducing conditions are expected to prevail in and around the container under the influence of the reducing groundwater, and consumption of any residual oxygen by reaction with the copper and steel container materials or with ferrous and organic material in the sealing materials. Under these conditions, the UO$_2$ would dissolve very slowly.

However, 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 $\alpha$, $\beta$ and $\gamma$ radiation emitted by the used fuel.
The fuel dissolution in the ISM-NF 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 (3-3).

$$C_{UO2} = \frac{A_{\text{fuel}}}{N_{\text{Symmetry}}} \left[ G_\alpha f_\alpha D_\alpha(t + t_c)^{a_\alpha} + G_\beta f_\beta D_\beta(t + t_c)^{a_\beta} + G_\gamma f_\gamma D_\gamma(t + t_c)^{a_\gamma} + R_{U\text{chem}} \right]$$  (3-3)

Where,

$$C_{UO2}$$ is the total used fuel dissolution rate [mol\(u\)/a];

$$A_{\text{fuel}}$$ 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];

$$G_\alpha, G_\beta, G_\gamma$$ are empirical rate constants for fuel dissolution in the presence of alpha, beta and gamma radiation fields, respectively [mol\(u\)/m\(^2\)/Gy];

$$f_\alpha, f_\beta, f_\gamma$$ 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 nuclide 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

$$R_{U\text{chem}}$$ is the chemical fuel dissolution rate, i.e., the dissolution rate of the fuel in the absence of radiolysis [mol\(u\)/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 (Shoesmith 2008).

The congruent dissolution release rate of species \(j\) from the UO\(_2\) fuel matrix in the failed container at time \(t\) is given by Equation (3-4).

$$F_{CD,UO2}^j(t) = (1 - f_{IRF,UO2}^j) \frac{I_{UO2}^j}{N_{\text{Symmetry}}} \frac{C_{UO2}(t)}{I_{UO2}^0} (t \geq t_F)(t \leq t_{UO2})$$  (3-4)

Where,

$$F_{CD,UO2}^j(t)$$ is the UO\(_2\) congruent dissolution rate of species \(j\) entering the container [mol/a]

$$f_{IRF,UO2}^j$$ is the fraction of species \(j\) release instantly from the UO\(_2\) matrix upon contact with water [-];

$$I_{UO2}^j$$ is the inventory of species \(j\) at time \(t\) in the UO\(_2\) fuel in a container [mol];

$$C_{UO2}(t)$$ is the UO\(_2\) matrix degradation rate in the failed container at time \(t\) [mol/a];
\( I_{0,UO2} \) is the initial inventory of UO\(_2\) in a container [mol];
\( t_F \) is the minimum time of container zone failures [a]; and
\( t_{UO2} \) is the time all UO\(_2\) has been dissolved [a] (see Equation (3-4)).

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 (3-5) has been satisfied.

\[
\frac{I_{0,U238}}{N_{Symmetry}} = \int_{t_F}^{t_{UO2}} F_{CD,U238}(t) \tag{3-5}
\]

Where,
\( I_{0,U238} \) is the initial inventory of U-238.

Equation 3-4 is solved numerically as the ISM-NF runs. U-238 is considered a suitable proxy for the UO\(_2\) matrix because it is the primary constituent of the fuel matrix and has a long half-life (4.468\( \times 10^9 \) years).

### 3.2.3 Instant Release from the Zircaloy Cladding

Similar to the UO\(_2\) matrix, a rapid release and a slow release process in the Zircaloy is modelled. The rapid or “instant” release applies to soluble species trapped in the outer surface oxide layer, which are assumed to be released more rapidly. The slow release applies to all species 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 3.2.4.

The rate of release of species \( j \) from the Zircaloy cladding by instant release is described by Equation (3-6). The instant release occurs via a smoothed rectangular function at the time of container failure.

\[
F^{j}_{IRF,Zr}(t) = \frac{f^{j}_{IRF,Zr}I^{j}_{Zr}\delta(t_F,t_{IRF})}{N_{Symmetry}} \tag{3-6}
\]

Where,
\( F^{j}_{IRF,Zr}(t) \) is the Zircaloy instant release rate of species \( j \) entering the container [mol/a];
\( f^{j}_{IRF,Zr} \) is the fraction of species \( j \) release instantly from the Zircaloy cladding upon contact with water [-];
\( I^{j}_{Zr} \) is the inventory of species \( j \) 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 minimum time of container zone failures [a]; and
\( t_{IRF} \) is the time over which the instant release is assumed to occur [a].
3.2.4 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 (3-7).

\[ C_{Zr} = k_{Zr}A_{Zr} \rho \]  

(3-7)

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 [m$^2$]; and
- $\rho$ is the density of Zircaloy [kg/m$^3$].

The congruent dissolution release rate of species $j$ from the Zircaloy cladding in the failed container at time $t$ is given by Equation (3-8).

\[ F_{CD,Zr}^j(t) = \frac{(1 - f^j_{IRF,Zr})I^j_{Zr}C_{Zr}}{N_{Symmetry}}(t \geq t_F)(t \leq t_{Zr} + t_F) \]  

(3-8)

Where,

- $F_{CD,Zr}^j(t)$ is the Zircaloy congruent release rate of species $j$ entering the container [mol/a];
- $f^j_{IRF,Zr}$ is the fraction of species $j$ release instantly from the Zircaloy upon contact with water [\ ];
- $I^j_{Zr}$ is the inventory of species $j$ at time $t$ in the Zircaloy cladding [mol/kg$_{Zr}$];
- $C_{Zr}$ is the Zircaloy cladding corrosion rate in the failed container at time $t$ [kg$_{Zr}$/a];
- $I_{0,Zr}$ is the initial mass of Zr in a cladding [kg$_{Zr}$];
- $t_F$ is the minimum time of container zone failures [a]; 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 (3-9).

\[ t_{Zr} = \frac{I_{0,Zr}}{C_{Zr}} \]  

(3-9)

Where,

- $I_{0,Zr}$ is the initial mass of Zr in the container [kg$_{Zr}$].
3.2.5 Model Source Term

The total source term for a given species is the sum of the instant and congruent release components for the fuel and the Zircaloy cladding and described by Equation (3-10).

\[
F_{Total}^j(t) = F_{IRF, UO_2}^j(t) + F_{CD, UO_2}^j(t) + F_{IRF, Zr}^j(t) + F_{CD, Zr}^j(t)
\]  

(3-10)

Where,

- \(F_{Total}^j(t)\) is the total source term for species \(j\) [mol/a];
- \(F_{IRF, UO_2}^j(t)\) is the UO\(_2\) instant release component defined in Equation (3-1) [mol/a];
- \(F_{CD, UO_2}^j(t)\) is the UO\(_2\) congruent release component defined in Equation (3-4) [mol/a];
- \(F_{IRF, Zr}^j(t)\) is the Zircaloy instant release component defined in Equation (3-6) [mol/a]; and
- \(F_{CD, Zr}^j(t)\) is the Zircaloy congruent release component defined in Equation (3-8) [mol/a].

The release of a given species into the container is defined as a flux boundary condition \(F_{Source}^i(t)\), proportional to the surface area over which the flux is applied and specified in mol/m\(^2\)/a. This flux, defined by Equation (3-10), is applied to the wasteform (source) boundary (see Figure 3-4).

\[
F_{Source}^i(t) = \frac{F_{Total}^i(t)}{A_{Model}}
\]  

(3-11)

Where,

- \(A_{Model}\) is the surface area within the ISM-NF model representing the wasteform (see Figure 3-4) over which the flux source term is applied [m\(^2\)].

Once species enter the ISM-NF model via the wasteform boundary, species can migrate through the container, engineered barrier system and excavation damages zone via advection and diffusion. Solubility limited species are treated as a special case and modelled using a fixed concentration at the wasteform boundary (see Section 3.2.6).
3.2.6 Solubility Limits, Precipitation, and Dissolution

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

Typically species 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 (3-9). 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 a species in the container well beyond the time after which the fuel has dissolved. This may be well beyond the times typically considered in postclosure safety assessments.

In the ISM-NF, the user specifies which species are modelled as solubility limited. Solubility limited species are modelled by setting the wasteform (source) boundary (see Figure 3-4) to a fixed concentration equal to the solubility limit of a given species (see Equation 3-11). Isotopes of a given element have the solubility limit of the element scaled by the isotopic abundance of the isotope.

\[
C_{\text{waste}}^j = f_{\text{iso}}^j(t)C_{\text{sol}}^k
\]  

(3-12)

Where,

\(C_{\text{waste}}^j\) is the solubility limited wasteform boundary concentration for species j;

\(f_{\text{iso}}^j(t)\) is the isotopic abundance of species j in element k at time t; and

\(C_{\text{sol}}^k\) is the solubility limit of element k.
3.3 Placement Room

The placement room portion of the ISM-NF model includes the container (Section 3.3.1), the engineered barrier system (Section 3.3.2) and Excavation Damaged Zone (Section 3.3.3). The primary processes modelled in the placement room portion of the ISM-NF model is the failure of the container (Section 3.3.4) and transport through the placement room components (Section 3.3.5).

3.3.1 Container

The reference container in the repository is designed to hold 48 used fuel bundles. The reference container concept has a corrosion-resistant copper coating and a structural steel inner vessel (Figure 3-5).

![Container Design](image)

Containers are designed to be robust and durable and intended to withstand the repository conditions essentially indefinitely. However the postclosure safety assessment model considers the possibility that some containers may fail; for example possibly from placement of undetected defective containers in the repository. The near field model assumes that once a container has failed there is sufficient water available to fill the container and to provide a connected pathway from the fuel to the bentonite surrounding the container. It is also assumed that the container boundary is generally maintained (i.e. the bentonite does not significantly expand into the container, nor does the container collapse as the internal and external pressure equilibrate), but the shell becomes effectively porous and open for outward radionuclide transport.

3.3.2 Engineered Barrier System

The engineered barrier system is composed primarily of highly compacted bentonite (HCB). HCB will be machined to hold and completely surround each used fuel container and is referred to as the buffer box (see Figure 3-6). Buffer boxes in the placement rooms will be spaced out with additional HCB spacer blocks.
Figure 3-6: Buffer Box

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 after over long periods of time the gap fill and HCB will homogenize, and reduce the distinct boundaries between the materials.

3.3.3 Excavation Damaged Zone

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 assumed to have higher transport properties than those in the intact host rock. The ISM-NF model includes two distinct zones outside the placement room. Typically the inner zone is used to represent a region of more permeable EDZ while the outer zone can be used to represent intact host rock or a broader less permeable EDZ zone.

3.3.4 Container Failure

The container model does not model the mechanism of container failure (e.g., corrosion). Instead the model assumes the container had failed at a defined failure time. Each container failure is assumed to occur in two failure zones (the hemi-head and the cylindrical container body) for a total of four possible failure zones. Each of the failure zones can fail at unique times or occur simultaneously. The failure zone is restricted to a thin boundary layer in the model representing the interface between the container and the bentonite (outside edge of the orange shaded area in Figure 3-7).

Failure of a container zone is modelled by transitioning the diffusion coefficient for all species from zero to the free water diffusion coefficient value over a predefined time. Figure 3-7 shows the container failure zones and an example of the function used to scale the diffusion coefficient with time.

Upon failure of any one of the zones, the wasteform is assumed to be in contact with groundwater. At this point, the interior of the container (orange shaded area in Figure 3-7) is available for transport of species release from the fuel source boundary (blue).
Transition of the diffusion coefficient are given by Equation (3-13). In each of the container zone boundary layers the diffusion coefficient is multiplied by a smoothed step function as defined below. Advective velocity in the container and failure zone layers is assumed to be zero.

\[
D_z^j(t) = f_z(t_z, w) D_{fw}^j
\]  

(3-13)

Where,

- \(D_z^j(t)\) is the time dependent diffusion coefficient for species \(j\), in zone \(z\) [m\(^2\)/a];
- \(f_z\) is the smoothed step function for the container failure zone, \(z\) (the smoothed step function is second order continuous and has a value of zero prior to time \(t_z\) and 1 for times greater than \(t_z + w\));
- \(t_z\) is the time at which zone \(z\) is assumed to fail [a];
- \(w\) is time over which the failure occurs (i.e., the width of the step function currently assumed to be 1 year); and
- \(D_{fw}^j\) is the free water diffusion coefficient for species \(j\).

### 3.3.5 Transport in the Placement Room

Once the container has failed, water accesses the fuel and species will enter the container as the wasteform degrades. From there, species are able to migrate out of the failed container, into the engineered barrier system, and through the excavation damaged zone to the model boundary. All materials in the placement room are assumed to be saturated and modelled as porous media. Though the container interior, bentonite and rocks have different material properties, transport of species within these materials are governed by the same advection-diffusion process (Equation (3-14)).
ISM-NF model solves for the concentration of a species at each position in the placement room (container, EBS and EDZ/Rock) as a function of time and space. Note that the advective velocity in the container is typically assumed to be zero and all material properties for the placement room domains (e.g., porosity, density) are assumed to be homogeneous and constant.

\[
(\theta_m + \rho_m K_{d_m}^j) \frac{\delta C_L^j}{\delta t} + \nabla \cdot (C_L^j \cdot u_m) = \nabla \left( \theta_m \tau_m^j D_{fw,m}^j \nabla C_L^j \right) + R_{\text{decay}}^j
\]  

(3-14)

Where,

- \( \theta_m \) is the porosity of material m [-];
- \( \rho_m \) is the density of material m [kg/m\(^3\)];
- \( K_{d_m}^j \) is the linear equilibrium sorption coefficient for species j in material m [m\(^3\)/kg];
- \( C_L^j \) is the liquid-phase (solute) concentration of species j [mol/m\(^3\)];
- \( u_m \) is the groundwater velocity vector (with x,y,z components) in material m [m/a];
- \( \tau_m^j \) is the tortuosity of species j in material m [-];
- \( D_{fw,m}^j \) is the free water diffusion coefficient of species j in material m [m\(^2\)/a];
- \( R_{\text{decay}}^j \) is the reaction term representing loss or creation of species j from radioactive decay and ingrowth (Equation (3-15)).

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 species j. If a species is a member of a chain, a second reaction represents ingrowth from the decay of the parent (species j-1). Both these reaction terms are defined in Equation (3-15).

\[
R_{\text{decay}}^j = (\theta_m + \rho_m K_{d_m}^{j-1}) \lambda_{j-1} C_{j-1}(t) - (\theta_m + \rho_m K_{d_m}^j) \lambda_j C_j(t)
\]  

(3-15)

Where,

- \( R_{\text{decay}}^j \) is the rate of change in concentration of species j due to radioactive decay of species j and ingrowth from the decay of the parent species j-1.

### 3.4 Model Boundary Conditions

There are three main boundary conditions applied in the ISM-NF model.

- The flux or fixed concentration source term applied along the model surface representing the wasteform (see Section 3.2.5, Section 3.2.6 and Figure 3-4);
- A zero concentration boundary condition applied to the external model boundary (see Figure 3-8a); and
- A no flux or symmetry boundary condition applied along the sides of the model (see Figure 3-8b).

Boundary conditions were selected to both optimize model performance (e.g., reduce the extent of the model domain) and be conservative.
Figure 3-8: (a) Zero Concentration Boundary Condition, (b) Symmetry Boundary Condition

3.5 Interface with the Geosphere Model

The near-field-to-geosphere model interface is defined at the buffer-EDZ interface and is highlighted in blue in Figure 3-9.

The output from the near field model is the surface integrated flux (i.e., total release rate) for each species crossing the bentonite-EDZ interface shown in Figure 3-9.

The total release of a species 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 species from the near field model is linearly scaled to represent the rate of a species entering the geosphere for any number of failed containers (see Equation (3-16)).
Figure 3-9: Buffer-EDZ Interface

\[ X_{GEO}^j(t) = X_{NF}^j(t) N_{symmetry} N_{Cont} f_{mol-kg}^j f_{a-s} \] (3-16)

Where,

- \( X_{GEO}^j(t) \) is the total release rate of species j entering the geosphere [kg/s];
- \( X_{NF}^j(t) \) is the nearfield release rate of species j through the bentonite-EDZ interface (boundary highlighted in blue in Figure 3-9) for one or two failed quarter containers [mol/a]. This is defined as the surface integral of the flux [mol/m²/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 [-];
- \( f_{mol-kg}^j \) is the conversion factor from mol to kg for species j [kg/mol]. The output from the ISM-NF model is converted to kg/s as these are the default units of the ISM-GEO model (HGS); and
- \( f_{a-s} \) is the conversion factor from years to seconds [s/a].

\[ X_{NF}^j(t) = \int \Phi_{NF}^j(t) \] (3-17)

Where,

- \( \Phi_{NF}^i \) is the flux (mol/m²/a) passing through the bentonite-EDZ interface (this is the boundary highlighted in blue in Figure 3-9).
4. ISM-GEO MODEL

4.1 Geosphere Model Overview

The ISM-GEO model (also referred to as the geosphere model) is developed using HydroGeoSphere (HGS) (Aquanty 2013). It represents the repository, the host rock, any fractures or aquifers present at the repository site and a domestic water well. The geosphere model determines the steady-state groundwater flow field and the subsequent species transport from the repository to the surface environment.

The ISM-GEO model has the full capabilities of HGS. These include:

- Complete hydrologic cycle modelling using detailed physics of surface and subsurface flow. The surface regime can be represented as 2D areal flow for the entire surface or as 2D runoff into 1D channels. The subsurface regime consists of 3D unsaturated/saturated flow. Both regimes naturally interact with each other through considerations of the physics of flow between them.
- Physically-based accounting of all components of a hydrologic cycle water budget.
- Accurate delineation and tracking of the water table position, taking into account flow in the unsaturated zone, delayed yield and vertical flow components.
- Handling of non-ponding or prescribed ponding recharge conditions.
- Automatic handling of seepage face conditions at the land-atmosphere interface.
- 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/temperature mixing within the water column in the well.
- Accommodation of wellbore storage.
- Arbitrary combinations of porous, discretely-fractured, dual-porosity and dual-permeability media for the subsurface.
- Capability of modelling non-reactive and reactive chemical species transport in associated surface and subsurface flow regimes.
- Calculation of temperatures in the surface and subsurface flow regimes as driven by air temperature and incoming solar radiation, accounting for land surface-atmospheric thermal interactions.
- Accurate handling of fluid and mass/thermal energy exchanges between fractures and matrix including matrix diffusion effects and solute/thermal energy advection in the matrix.
- Straight or branching decay chains representing degradation reactions.

This version of the ISM-GEO model includes the following HGS features:

- 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 equivalent porous media (EPM) approach; and
- A domestic well.

In future versions of the ISM-GEO model, any of the HGS features listed above may be included through changes to the HGS user options and input files. In this report, the basic HGS theory as
applicable to the current ISM-GEO model is discussed. The theory for all HGS features and numerical implementation is given in Aquanty (2013).

While not theory per se, the most critical component of the ISM-GEO model are the model geometry, mesh, and materials defined by the user to ensure the ISM-GEO model is reflective of the repository and repository site. The example version the ISM-GEO model described here is based on the FRAC3DVS-OPG (Therrien et al. 2010) Rooms-Only Repository-Scale Model from the Sixth Case Study (NWMO 2017).

Figure 4-1 shows an example of an ISM-GEO model geometry. In this example four unique rock layers: surface (teal), shallow (green), intermediate (light green) and deep (orange) rocks are included in the model. Major fractures are modelled as regions of equivalent porous media and shown in dark blue. The individual repository placements rooms are represented (pink). However, shafts and other repository features are not included. The well is located near bottom-right edge of the bottom-centre panel of the repository (not shown due to cut-away).

![Figure 4-1: Example of ISM-GEO Model Geometry](image)

This example model covers a 4.0 x 5.0 km rectangular domain. The model has 93 layers vertically with 6.45 million nodes and 6.33 million elements in total. More detailed descriptions of this model are available in NWMO (2017). It is expected that an ISM-GEO model reflective of potential real-world repository sites will be developed in the future.

Input to the ISM-GEO model is a flux source term as determined by the ISM-NF model (Section 3.5, Section 4.2), material properties (e.g., porosity, density, and permeability), transport properties (e.g., diffusion coefficients, sorption coefficients) and decay properties (e.g., half-lives, branching ratios).
The output from the geosphere model is the integrated flux to the domestic water well and a number of user-defined surface discharge areas (Section 4.4).

4.2 Geosphere-Near Field Interface

The defined interface between the ISM-NF and ISM-GEO models is the interface between the engineered barrier system and the excavation damaged zone. The output from the near-field model described in the previous chapter is the transport (in kg/s) of a species as it crosses that threshold scaled to represent one or several failed containers (see Section 3.5). In turn, the geosphere model applies that transport rate as a source term. The geosphere model source terms is evenly distributed across several source nodes defined by the user.

Figure 4-2 shows how source nodes (fuchsia nodes) are applied in the ISM-GEO model. The rectangular green volume represents a portion of a placement room, and the translucent purple volume is the surrounding EDZ. The fuchsia nodes represent the source nodes over which the near field source term is uniformly applied. The source nodes are distributed across a section of a placement room representing 10 container placement positions.

Since the ISM-NF model models release from the containers and transport through the engineered barrier system, none of these features are represented in detail in the ISM-GEO model. Furthermore, transport within the placement room surrounded by the source nodes is turned off (i.e. species cannot travel back into the placement room). Transport in other portions of the placement room outside the source nodes, and in the surrounding rock mass, is allowed.

![Figure 4-2: Geosphere - Near Field Model Interface](image)

4.3 Geosphere Model Theory

The following sections summarize the groundwater flow and species transport theory specific to the ISM-GEO geosphere model. As noted in Section 4.1, the ISM-GEO model uses only some of the HGS available features. A detailed description of the complete HGS theory and numerical implementation is available in Aquanty (2013).
### 4.3.1 Subsurface Flow

Subsurface flow describes the movement of groundwater through the geosphere. For the ISM-GEO model, the system is assumed to be a fully saturated porous medium. 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 used to describe three-dimensional transient subsurface flow in a variably-saturated porous medium in HGS:

\[
- \nabla \cdot (w_m q) + \sum I'_{ex} \pm Q = w_m \frac{\partial}{\partial t} (\theta_m S_w)
\]

(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);

\(I'_{ex}\) 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.

\(\theta_m\) is the porosity of the medium \([-]\); and

\(S_w\) is the water saturation \([-]\), assumed to be 1 or fully saturated in ISM-GEO.

\[
q = -K \cdot k_r \nabla (\psi + z)
\]

(4-2)

Where,

\(k_r\) represents the relative permeability of the medium \([-]\);

\(\psi\) 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)

\[
K = \frac{\rho g}{\mu} k
\]

(4-3)

Where,
\( g \) is the gravitational acceleration \([\text{m/s}^2]\);
\( p \) is the density of water \([\text{kg/m}^3]\);
\( \mu \) is the viscosity of water \([\text{kg/m/s}]\); and
\( k \) is the permeability tensor of the permeable media \([\text{m}^2]\).

### 4.3.2 Subsurface Flow in Fractures and Aquifers

HGS and therefore ISM-GEO is capable of modelling discrete fractures; however this feature is not currently used in ISM-GEO. Fractures and fractured rock masses are represented by equivalent porous media (Section 4.3.1) with more conductive material properties.

### 4.3.3 Subsurface Flow in the Well

Groundwater wells is assumed to be present in the ISM-GEO model in most simulations and used to provide water for domestic use by humans assumed to be living on the surface above the repository site. Generally, the length of the well can be assumed to be much larger than the cross-sectional area of the well casing. With this assumption, 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 (4-4), (4-5) and (4-6).

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

\[
\frac{\partial}{\partial s} \left( \pi r_w^2 \frac{\rho g \partial h_w(s)}{8 \mu \partial s} \right) + Q_w \delta(s - s_p) + \Gamma_{pm \rightarrow w} = n r_w^2 s_{sw} \frac{\partial h_w(s)}{\partial t} \quad (4-5)
\]

\[
s_{sw} = \rho g \beta \quad (4-6)
\]

Where,

- \( Q_{1D} \) is the fluid flux along the one-dimensional well axis \([\text{m}^3/\text{s}]\);
- \( r_w \) is the well radius \([\text{m}]\);
- \( \rho \) is the density of water \([\text{kg/m}^3]\);
- \( g \) is the gravitational acceleration \([\text{m/s}^2]\);
- \( \mu \) is the viscosity of water \([\text{kg/m/s}]\);
- \( h_w(s) \) is the well hydraulic head at position \( s \) along the well axis \([\text{m}]\);
- \( s \) is the well coordinate along the well axis \([-]\);
- \( Q_w \) is the well discharge (or recharge) per unit length \([\text{m}^2/\text{s}]\);
- \( \Gamma_{pm \rightarrow w} \) is the fluid exchange between the surrounding porous medium (pm) and the well (w) \([\text{m}^3/\text{s}]\). \( \Gamma_{pm \rightarrow w} \) is defined by equation (4-7) assuming a flux continuity between the well and surrounding medium;
- \( s_{sw} \) is the specific storage coefficient for a fluid filled borehole \([\text{m}^{-1}]\); and
- \( \beta \) is the compressibility of water \([\text{m} \cdot \text{s}^2/\text{kg}]\).
\[
I_{pm-w} = -2\pi r_w(k_r)_{exch(pm,w)} K_{exch(pw,w)} \frac{h_w(s) - h}{l_{exch(pm,w)}}
\]  

(4-7)

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].

**4.3.4 Transport in Saturated Porous Media**

Three-dimensional transport of solutes in a variably-saturated porous matrix is described by the following equation:

\[
-\nabla \cdot w_m (q C_j - \theta_m S_w D V C_j) + w_m \theta_m S_w R_{j-1} \lambda_{j-1} C_{j-1} + \sum \Omega_{ex} \pm Q_c = w_m \left( \frac{\partial (\theta_m S_w R_j C_j)}{\partial t} + \theta_m S_w R_j \lambda_j C_j \right)
\]

(4-8)

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/m³] of species \(j\);

\(\theta_m\) is the porosity of the medium [-];

\(S_w\) is the water saturation [-], assumed to be 1 or fully saturated in ISM-GEO;

\(D\) is the hydrodynamic dispersion tensor [m²/s] given by Equation (4-10);

\(\lambda_j\) is a first-order decay constant [s⁻¹] of species \(j\). The subscript “\(j-1\)” designates parent species for the case of a decay chain;

\(\Omega_{ex}\) represents the mass exchange rate of solutes per unit volume [kg/m³/s] between the subsurface domain and all other types of domains supported by the model (e.g., the well);

\(Q_c\) represents solute exchange from boundary conditions [kg/m³/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 species \(j\) and is given by Equation (4-9).
\[ R_j = 1 + \frac{\rho_b}{\theta_m S_w} K d_j \]  

(4-9)

Where,

- \( \rho_b \) is the bulk density of the porous medium [kg/m\(^3\)]; and
- \( K d_j \) is the linear adsorption isotherm [m\(^3\)/kg] of species j.

\[ \theta_m S_w D = (\alpha_l - \alpha_t) \frac{qq}{|q|} + \alpha_t |q| l + \theta_s S_w \tau D_f^j_w l \]  

(4-10)

Where,

- \( \alpha_l \) and \( \alpha_t \) are the longitudinal and transverse dispersivities [m], respectively;
- \( |q| \) is the magnitude of the Darcy flux;
- \( \tau \) is the matrix tortuosity [-];
- \( D_f^j_w \) is the free-solution diffusion coefficient of species j [m\(^2\)/s]; and
- \( l \) is the identity tensor.

### 4.3.5 Transport in the Well

One-dimensional solute transport along the axis of a well is described by:

\[ -\nabla \cdot \pi r_s^2 (q_w C_{w,j} - S_{ww} D_w^j \bar{\nabla} C_{w,j}) + \pi r_s^2 \lambda_j C_{w,j-1} - \pi r_s^2 \lambda_j C_{w,j} - Q_w (C_{w,j} - C_{w,\text{inj},j}) \delta(l - l') - \pi r_s^2 \Omega_w = \pi r_s^2 \frac{\partial C_{w,j}}{\partial t} \]  

(4-11)

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;
- \( D_w \) is the dispersion coefficient in the well given by Equation (4-12);
- \( \lambda \) is a first-order decay constant [s\(^{-1}\)]. The subscript “j-1” designates parent species for the case of a decay chain;
- \( Q_w \) is the well discharge (or recharge) per unit length [m\(^2\)/s] applied at location \( l' \);
- \( C_{w,\text{inj},j} \) is the concentration of species 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
- \( \Omega_w \) 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 equal to Equation (4-12):
\[ D_f^j = \frac{r_s^2 q_w^2}{48 D_{fw}} + D_f^j \]  

(4-12)

Where,

\( D_f^j \) is the free-solution diffusion coefficient of species j [m²/s].

### 4.3.6 Boundary Conditions

#### 4.3.6.1 Flow Boundary Conditions

Boundary conditions for subsurface flow in HGS include the following: first-type (Dirichlet) boundaries of prescribed hydraulic or pressure head, areal infiltration or recharge, source/sinks, evaporation, seepage faces, free-drainage and drain nodes. The boundary conditions can also be allowed to vary in time.

When HGS is used to solve fully coupled subsurface and surface flow, the areal recharge boundary for subsurface flow is not required since the solution to the interacting system determines the subsurface recharge.

#### 4.3.6.2 Transport Boundary Conditions

Boundary conditions for solute transport in HSG include the following: first-type (prescribed concentration), second type (prescribed mass flux) or third-type (prescribed total flux) boundary conditions and can be input as time-dependent quantities.

#### 4.3.6.3 ISM-GEO Boundary Conditions

In the ISM-GEO model, all model top surface nodes are assigned fixed head boundary condition at topographic elevations. Model bottom boundary conditions are set to zero flow. Fixed head boundary conditions at vertical model sides are input to ISM-GEO, and usually interpolated from head fields calculated with another larger-scale model of the site. Head values for the example geosphere (with no well pumping) are shown in Figure 4-3.

Transport boundary conditions in the ISM-GEO model are time-variant mass fluxes (provided by ISM-NF) applying to the source nodes shown in Figure 4-2. In essence this results in flux of species to the surface or through the sides of the model domain together with groundwater flow.
4.4 Interface with the Biosphere Model

The flow portion of the ISM-GEO model describes how the water moves through the system and the transport portion shows how, given that groundwater flow field, species migrate through the geosphere environment. Of primary concern to postclosure safety assessment is the transport of species to the surface environment.

In order to estimate species transport to the surface, the user defines areas on the surface over which the flux of a species (kg/m²/a) is integrated (this is similar to how the ISM-NF model integrates the flux through the outer boundary of the placement room). Typically, the groundwater flow field directs species to localized areas at the surface. In particular, surface discharges generally correspond with surface water features (wells, lakes, rivers, wetlands) and topographic lows. The boundaries for these features are typically defined by the user, based on the modelling results.

Figure 4-4 shows the advective transport pathways from particles released from the repository in the ISM-GEO example model. Fuchsia points represent locations where particles reach the discharge points. Note that the particle tracks shown in Figure 4-4 only represent the advective component of transport. There is a diffuse plume following the advective flow path and reaching the surface. This means that discharge to the surface is not concentrated at a singular point but distributed over an area.

Figure 4-5 shows a top down view of the example model surface with the repository footprint projected onto the surface. The flux to the surface is distributed across five primary discharge areas. A domestic water well (black circle), the central wetland, the west river, the east river, and the south river. The cluster of discharge points in each discharge area corresponds to the discharge points in Figure 4-4. The boundary of each surface discharge area is defined by the user and corresponds to area over which the diffusive plume intersects the surface.

Transport to a given surface discharge location is determined by integrating the flux of a given species over the corresponding defined surface area. Transport for each discharge area and
species is then passed to the biosphere model. The type and number of surface discharges will depend on the repository site and should reflect site specific features.

Figure 4-4: Advective Transport Pathways in Example Model

Figure 4-5: Geosphere - Biosphere Model Interface in Example Model Showing Repository Footprint Projected to Surface and Advective Discharge Points
5. ISM-BIO MODEL

The ISM-BIO model (also referred to as the biosphere model) describes the movement of radioactive and non-radioactive species in the surface environment after release from the geosphere, and the consequent radiological dose and non-radiological consequences to a reference human individual.

The ISM-BIO model is implemented in AMBER, which is a compartment modelling software developed by Quintessa Ltd (Quintessa, 2018). AMBER takes into account the ingrowth and decay of radionuclides in each compartment, and therefore the equations related to these processes are not presented here. The model assumes that compartments are instantaneously homogenously mixed as species are transferred from one compartment to the next.

5.1 Biosphere Model Overview

The biosphere model is developed to evaluate the long-term postclosure environmental and health impacts of a deep geologic repository in a temperate climate state. It estimates the consequences to a hypothetical reference human group 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 biosphere model is intended to be a simplified and largely generic representation of the biosphere. The ISM-BIO model allows for up to six unique surface discharge locations. Two possible terrestrial discharge locations (e.g., garden or forage fields), three possible aquatic discharge locations (e.g., lakes, rivers, or wetlands) and a well discharge. Depending on the site being assessed, the type and number of surface features can be manipulated (through input data) to be representative of a variety of sites. For example, a site including a lake, a river and wetland connected in sequence or three rivers following into one another can be achieved through surface water parameter data.

Input to the ISM-BIO model from the geosphere model is described in Section 4.4 and Section 5.2 and consists of series of transport rates to defined surface discharge locations. Transport rates from the geosphere surface discharge areas are applied as source terms to compartments representing surface features (e.g., surface waters, soils) in the biosphere model.

Species can migrate through environmental media in the biosphere via a number of transfer pathways. An important distinction is made in the ISM-BIO with some media being represented as compartments and others represented as components. Compartments include things like surface waters and soils. Species transferred between compartments represent migration from one compartment to the next via a defined transfer. Components represent features in the biosphere whose concentration is estimated assuming an equilibrium with a specific biosphere compartment. Examples of components in the biosphere include the atmosphere and sediments. The concentration in atmosphere or sediments are estimated assuming an equilibrium exchange with the soil and surface water features. Figure 5-1 illustrates the ISM-BIO model compartments and the transfers between them. Note that Figure 5-1 also includes a sink as a compartment. This represents loss from the local biosphere due to processes like outflow, burial into sediments and volatilization.
Figure 5-1: Transfer Model between Biosphere Compartments

Figure 5-2 shows the connection between ISM-BIO model compartments and components including environmental media and biota. Note that the well in the ISM-BIO model is not expressly represented as a compartment or a component but rather a source applied to both compartments and components.

Figure 5-2: Connection between Model Compartments and Components
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. Dose pathways included in the ISM-BIO model are shown in Figure 5-3.

Dose pathways depend on the lifestyle of the critical group assumed to be living at site. The ISM-BIO model evaluates the consequences for two different lifestyles: a self-sufficient farming lifestyle and a hunter-gatherer lifestyle. The lifestyle of the exposed critical groups are based on human behaviour using conservative, yet reasonable, assumptions. For example, members of the critical groups are assumed to live their entire lives at the repository site, having access to all those parts of the biosphere that are potentially contaminated.

User options to change of modify the lifestyle, receptor and key biosphere characteristics include:

1. The lifestyle of the critical group (hunter-gather or farmer),
2. The age group of the receptor (infant, child or adult),
3. The main surface water feature that is used for domestic and irrigation purposes (option of a lake, river or a wetland selected by the user), and
4. The well use (on or off).

The equations that define the ISM-BIO model are based on the CSA N288.1-14 model (CSA 2014). However, the intended use of CSA N288.1-14 is somewhat different from a repository postclosure safety assessment. The CSA N288.1-14 is intended to provide guidelines for calculating derived release limits for airborne and liquid effluents for normal operations of nuclear facilities, and therefore the source of the contaminations is different (i.e., airborne stack release and liquid effluent from a facility vs. geosphere discharge). The ISM-BIO model includes many of the CSA N288.1-14 processes; notable exceptions are release from an airborne stack, atmospheric dispersion and release of liquid effluent to surface water.

Another key difference between ISM-BIO and CSA N288.1-14 is that CSA N288.1-14 is not a dynamic model. That is, it assumes steady release and an equilibrium between biosphere components. The ISM-BIO model calculates concentration of species in soil and surface waters, by allowing for dynamic transfer of species between media. This is to accommodate a time-varying release rate into the biosphere from the geosphere. Concentration in other biosphere components are calculated assuming steady release and equilibrium between components as in CSA N288.1-14. All dose pathways in CSA N288.1-14 are included in the ISM-BIO model.
Output from the geosphere model consists transport of species (flux integrated over a defined discharge area) reaching the surface in the geosphere model (see Section 4.4). The biosphere model uses this as input to the biosphere compartments and components. The ISM-BIO allows for connection of six biosphere features; 3 surface water features, 2 soils and a well. Figure 5-4 provides an illustration of the geosphere-biosphere model interface. In Figure 5-4 the terms $X_{A1}$, $X_{A2}$, and $X_{A3}$ represent the source term to the three surface water compartments in the biosphere model equal to the integrated flux from three discharge areas, $A_1$, $A_2$, and $A_3$, in the geosphere model. Similarly, $X_{T1}$ and $X_{T2}$ represent the source term to the two subsoil compartments in the biosphere model equal to the integrated flux from two discharge areas $T_1$ and $T_2$ in the geosphere model. $X_{W}$ represents the source term to the well in the biosphere model equal to the flux from the well in the geosphere model. As noted earlier, the well is not modelled as a compartment in the biosphere model but rather a source to other compartments and components.
In general,

\[ X_s^j(t) = \int \Phi^{j}_{GEO,D}(t)f_{kg-mol}f_{s-a} \]  

(5-1)

Where,
- \( X_s^j(t) \) is the transport into the biosphere surface feature \( s \) for species \( j \) in [mol/a];
- \( \Phi^{j}_{GEO,D} \) is the flux from the geosphere for discharge \( D \) and species \( j \) within surface feature \( s \) in [kg/m\(^2\)/s];
- \( f_{kg-mol} \) is the conversion factor from kg to mol for species \( j \) [mol/kg]; and
- \( f_{s-a} \) is the conversion factor from seconds to years [a/s].

### 5.3 Soil Concentration

#### 5.3.1 Overview

Figure 5-5 from Goodwin et al. (1994) illustrates the general processes included in the soil modelling.
Figure 5-5: Soil Transport Processes

The model assumes that species enter the subsoil from the geosphere model via contaminated groundwater. From the subsoil, species can move up into the surface soils. Two field types (garden, forage field) are considered. Both the garden and the forage fields have areas associated with them (determined in Section 5.3.2 and 5.3.3) as do the soil discharge areas in the geosphere model (see Section 5.2). However these areas do not necessarily correspond with one another. For conservatism, the soil discharge areas in the geosphere are typically selected to be much larger than the field areas in the biosphere. The integrated transport rate from the geosphere model into the soil discharge areas is then directed into the respective subsoil in the biosphere model. For clarity, one geosphere soil discharge area is linked to the biosphere garden, and the other geosphere soil discharge area is linked to the biosphere forage field.

The garden is assumed to be used to grow vegetables and fruit for consumption by the farmer, whereas the forage field is assumed to grow grain crops such as wheat for consumption by the farmer and the farmer’s livestock, or wild plants for consumption and general pasture for consumption by wild game for the hunter-gatherer.

It is assumed that all fields have the same soil type and experience the same annual precipitation. The irrigation demand per square metre of irrigated soil is then considered to be the same for the garden and the forage field. Because the fields have different areas, the annual volume of water required to irrigate the respective fields will vary between fields.

5.3.2 Garden Field
5.3.2.1 Self-Sufficient Farmer Lifestyle

The garden is assumed to be just large enough to supply the farmer’s family with the required amount of potatoes, fruits and vegetables. For the purposes of calculating the field area, the
model assumes that the ingestions rates of potatoes, fruits and vegetables correspond to those of the adults. Therefore, the following equation describes the area of the garden field:

\[
A^f = \frac{N_{\text{crit}}}{f^{f_{\text{crop}}}} \sum_{p \in f} \frac{R_{\text{ing},p}^{a,l}}{Y_p}
\]

with \( f = \text{garden}, l = \text{farmer}, \) and \( a = \text{adult} \)

Where,

- \( A^f \) is the area of field \( f \) [m^2];
- \( N_{\text{crit}} \) is the number of people in the critical group [\( - \)];
- \( R_{\text{ing},p}^{a,l} \) is the ingestion rate of plant \( p \) for age group \( a \) and lifestyle \( l \) [kg_{fw}/a];
- \( Y_p \) is the plant yield density for plant \( p \) [kg_{fw}/m^2_{soil}];
- \( f^{f_{\text{crop}}} \) is the cropping frequency of field \( f \) [a^{-1}]; and
- \( p \in f \) refers to the different plants that are within field \( f \).

The farmer’s field is preferentially irrigated using well water, as long as there is water in the well once the domestic water needs have been met. Otherwise, surface water is used to irrigate the garden field. The hunter-gatherer is not assumed to use a garden field.

5.3.2.2 Hunter-Gatherer Lifestyle

A garden field is not used in the hunter gatherer lifestyle.

5.3.3 Forage Field

5.3.3.1 Self-Sufficient Farmer Lifestyle

The forage field is made large enough to support the farmer’s domestic animals with forage crops and to grow grains for human (and domestic livestock) consumption. For the purposes of calculating the field area, the model assumes that the ingestions rates correspond to those of the adults. Therefore, the area of the forage fields that supplies the required amount of forage and grains to support the critical group is calculated as follows:

\[
A^f = \frac{N_{\text{crit}}}{f^{f_{\text{crop}}}} \left( \frac{R_{\text{ing},p}^{a,l}}{Y_p} \right) + \sum_{l_{s}} \frac{N_{l_{s}}^{f_{\text{crop}}}}{f^{f_{\text{crop}}}} \left( \frac{R_{\text{ing},\text{feed}}^{l_{s}}}{DW_p \cdot Y_{\text{feed}}} \right)
\]

with \( f = \text{forage}, p = \text{grain}, l = \text{farmer} \) and \( a = \text{adult} \)

Where,

- \( A^f \) is the area of field \( f \) [m^2];
- \( N_{\text{crit}} \) is the number of people in the critical group [\( - \)];
- \( R_{\text{ing},p}^{a,l} \) is the ingestion rate of plant \( p \) for lifestyle \( l \) and age group \( a \) [kg_{fw}/a];
- \( Y_p \) is the plant yield density of plant \( p \) [kg_{fw}/m^2_{soil}];
- \( l_{s} \) refers to livestock (dairycattle, beefcattle, pig, lamb or chicken);
- \( N_{l_{s}} \) is the number of livestock \( l_{s} \) [\( - \)].
\( R_{\text{ing,feed}} \) is the livestock ingestion rate of feed [kg_{dw}/a];
\( DW_p \) is the dry/fresh weight ratio of plant type p [kg_{dw}/kg_{fw}]
\( Y_{\text{feed}} \) is the forage feed yield density [kg_{fw}/m^2_{soil}]; and
\( f_{\text{crop}} \) is the cropping frequency of field f [a^{-1}].

The number of livestock of each type, which is rounded up to the nearest integer, is calculated from Equation (5-4):

\[
N_{ls} = \frac{N_{\text{crit}} \cdot R_{\text{ing,ls}}^a}{Y_{ls}}
\]

with \( a = \text{adult} \) and \( l = \text{farmer} \)

Where,
\( N_{ls} \) is the number of livestock ls [-];
\( N_{\text{crit}} \) is the number of people in the critical group [-];
\( R_{\text{ing,ls}}^a \) is the ingestion rate of livestock ls for age group a and lifestyle l [kg_{fw}/a]; and
\( Y_{ls} \) is the average dressed yield of livestock ls [kg_{fw}/a].

The forage field is assumed to be irrigated with surface water in the farmer lifestyle.

5.3.3.2 Hunter-Gatherer Lifestyle

In the hunter-gatherer lifestyle, the forage field is a source of contamination for wild plants and animals. For conservatism, the size of the forage field in the hunter-gatherer lifestyle is assumed to be the same size as that of the self-sufficient farmer, even though the hunter-gatherer is not assumed to raise livestock or domestic crops. Wild plants and animals could realistically be distributed over a much larger area than a forage field associated with a farmer lifestyle. However, it is plausible that a particular species of plant or animal would remain local to a specific contaminated biosphere location. Seasonal or other migratory occupancy factors are not accounted for in the ISM-BIO model.

In the hunter-gatherer lifestyle, the forage field is not irrigated.

5.3.4 Sub-Soil

The discharge rates from the deep geosphere to the biosphere are determined by the geosphere model and described in Section 5.2.

Many processes affect the flow from the sub-soil to the surface soil and vice versa. These processes depend on the weather, the soil properties and the depth of the soils. Processes include:

- Infiltration – the process by which rainfall, snowmelt or irrigation enters the soil through ground surface. Infiltration occurs closer to the surface of the soil. The rate of infiltration is influenced by the hydraulic properties of the soil and the depth to the water table.
• 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.
• Bioturbation – considers the concept that earthworms, burrowing animals and plant roots could bring species up from the subsoil.
• Advection – in soils refers to the mass movement of water that is caused by any process (typically a hydraulic head gradient) that moves water in a vertical or horizontal direction. Runoff is an example of advection.
• Diffusion – in surface soils, diffusion may be a significant mechanism causing the migration and redistribution of radionuclides in soils in the absence of a hydraulic gradient.

All of these processes are depth-limited; the deeper the contamination, the less effectively 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 species 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 in the future.

5.3.5 Surface Soil

There are four routes of entry evaluated for species entering the surface soil in addition to ingrowth from radioactive decay. These are irrigation with well water, irrigation with surface water, upflow from sub-soil (Section 5.3.4), and deposition from the atmosphere.

5.3.5.1 Irrigation from Well Water

Well water is used to irrigate the garden field, as this provides a direct path for geosphere water to reach the human food supply. This transfer is only assumed in the farming lifestyle under the condition that the well capacity is large enough for garden irrigation after domestic water needs have been met. The following equations, which rely on the proportion of well water that is used to irrigate the garden field, describe the transfer rate as follows:

If the well is in use and the farming lifestyle is being modelled, then:

\[ \varphi_{irr}^{jI}(t) = X_{well}^{j}(t) \cdot f_{well}^{irr}I \cdot \frac{Q_{irr}}{Q_{well}} \]  \hspace{1cm} (5-5)

Where,

\[ \varphi_{irr}^{jI}(t) \] is the source flux of species \( j \) from the well to the garden field surface soil [mol/a];
\[ X_{well}^{j}(t) \] is the discharge rate of species \( j \) from geosphere to the well [mol/a];
\[ f_{well}^{irr}I \] is the fraction irrigation water that is taken from the well (defined below) for lifestyle \( I \);
\[ Q_{well} \] is the total well demand [m\(^3\)water/a]; and
\[ Q_{irr} \] is the irrigation water demand [m\(^3\)water/a] as defined in Equation (5-24).
For \( l = \text{farmer} \):

\[
f_{\text{well}}^\text{irr,1} = \begin{cases} 
1 & \text{If } Q_{\text{cap}} \geq Q_{\text{irr}} + Q_{\text{dom}} \text{ and well is in use} \\
\frac{Q_{\text{cap}} - Q_{\text{dom}}}{Q_{\text{irr}}} & \text{If } Q_{\text{dom}} < Q_{\text{cap}} < Q_{\text{dom}} + Q_{\text{irr}} \text{ and well is in use} \\
0 & \text{If } Q_{\text{cap}} \leq Q_{\text{dom}} \text{ or well is not in use}
\end{cases}
\] (5-6)

Where,

- \( Q_{\text{cap}} \) is the annual well capacity \([\text{m}^3\text{water}/\text{a}]\)
- \( Q_{\text{dom}} \) is the domestic water demand \([\text{m}^3\text{water}/\text{a}]\)
- \( Q_{\text{irr}} \) is the irrigation water demand \([\text{m}^3\text{water}/\text{a}]\).

For \( l = \text{hunter-gatherer} \):

\[
f_{\text{well}}^\text{irr,1} = 0
\] (5-7)

For the hunter-gatherer, the flux from the well to the garden is always zero.

5.3.5.2 Irrigation from Surface Water

For the farmer, if there is still water in the well after the domestic water needs have been met, the rest of the well supply is used for irrigating the garden field. The remaining irrigation water needs are sourced from the main surface water feature. The forage field is assumed to be irrigated by the main surface water feature by the farmer. The hunter-gatherer is not assumed to irrigate either fields or to grow a garden.

The rate of transfer from surface water features to fields due to irrigation is as follows:

\[
\lambda_{\text{irr}}^{\text{sw,1,f,j}}(t) = \frac{N_{\text{sw}}^j(t) \cdot R_{\text{irr}}^f \cdot A^f \cdot f_{\text{sw,1,f}}^{\text{irr,1}} \cdot \delta_{\text{msw}}}{V_{\text{sw}}}
\] (5-8)

Where,

- \( \lambda_{\text{irr}}^{\text{sw,1,f,j}}(t) \) is the irrigation transfer rate for each surface water feature \( \text{sw} \) to the soil of field \( f \) for lifestyle \( l \) and species \( j \) \([\text{mol/a}]\);
- \( N_{\text{sw}}^j(t) \) is the amount of species \( j \) in surface water feature (compartment) \( \text{sw} \) as determined by AMBER \([\text{mol}]\);
- \( R_{\text{irr}}^f \) is the irrigation rate of field \( f \) \([\text{m}^3\text{water}/\text{a}/\text{m}^2\text{soil}]\);
- \( A^f \) is the area of field \( f \) \([\text{m}^2\text{soil}]\);
- \( V_{\text{sw}} \) is the volume of the surface water feature \( \text{sw} \) \([\text{m}^3\text{water}]\);
- \( f_{\text{sw,1,f}}^{\text{irr,1}} \) is the fraction of garden irrigation water for lifestyle \( l \) that is taken from the surface water feature \( \text{sw} \) for field \( f \) \([-]\); and
δ_{msw} is a switch which defines the user specified main water feature [-]. Its value is 1 when applied to the main surface water feature and 0 when applied to other surface water features.

For the farmer, \( f_{\text{sw},f}^{\text{irr,l}} \) is calculated as follows:

\[
f_{\text{sw},f}^{\text{irr,l}} = 1 - f_{\text{well}}^{\text{irr,l}}
\]

Since the hunter-gatherer does not irrigate, \( f_{\text{well}}^{\text{irr,l}} \) for the hunter-gatherer is zero.

5.3.5.3 Leaching

Leaching is the downward movement of species into the soil by infiltrating water. The species are lost from the surface soil, but are assumed to quickly move down to the water table and from there to the surface water features. Clause 6.3.6.1 of CSA (2014) recommends the following equation for the leaching rate:

\[
\lambda_{\text{leach}}(t) = \frac{N_f^j(t) \cdot q_{\text{infil}} \cdot f_{\text{wat}}^j \cdot \delta_{\text{msw}}}{\theta_w \cdot Z_s} \tag{5-10}
\]

Where,

- \( \lambda_{\text{leach}}(t) \) is the leaching rate of species \( j \) from surface soil \( f \) [mol/a];
- \( N_f^j(t) \) is the amount of species \( j \) in surface soil (compartment) \( f \) as determined by AMBER [mol];
- \( q_{\text{infil}} \) is the net infiltration rate of water through the soil [m³/m²/a] (Equation (5-12));
- \( Z_s \) is the depth of the surface soil layer [m];
- \( \theta_w \) is the soil water content [m³_water/m³_soil];
- \( \delta_{\text{msw}} \) is a switch which defines the user specified main water feature [-]. Its value is 1 when applied to the main surface water feature and 0 when applied to other surface water features; and
- \( f_{\text{wat}}^j \) is the fraction of species \( j \) in soil in the water phase (i.e., not sorbed), which is given by Equation (5-11):

\[
f_{\text{wat}}^j = \frac{\theta_w}{\theta_w + K_{d_{\text{soil}}}^j \cdot \rho_{\text{soil}}}
\]

Where,

- \( \theta_w \) is the soil water content [m³_water/m³_soil];
- \( K_{d_{\text{soil}}}^j \) is the solid-to-liquid partition coefficient for soil for species \( j \) [m³_water/kg_soil-dw];
- \( \rho_{\text{soil}} \) is the soil density [kg_soil-dw / m³_soil].
CSA (2014) 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 2014), thus:

$$q_{\text{infil}} = \frac{P_{\text{tot}} - R_T}{2} \text{ (if } P_{\text{tot}} > R_T, \text{ otherwise 0)} \quad (5-12)$$

Where,

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

5.3.5.4 Erosion

Erosion of the surface soil is characterized by an erosion rate $ER$, and the associated erosive transfer rate $\lambda_{er}$ of species out of the soil layer and into the surface water is characterized by Equation (5-13) (Clause 6.3.4.1 of CSA 2014):

$$\lambda_{er}^j(t) = \frac{N_f^j(t)ER(1 - f_{\text{wat}})\delta_{\text{msw}}}{\rho_{\text{soil}} \cdot Z_s} \quad (5-13)$$

Where,

- $\lambda_{er}^j(t)$ is the erosive transfer rate of species $j$ [$a^{-1}$];
- $N_f^j(t)$ is the amount of species $j$ in surface soil (compartment) $f$ as determined by AMBER [mol];
- $ER$ is the erosion rate [$kg_{dw}/m^2_{soil}/a$];
- $\rho_{soil}$ is the soil density [$kg_{dw}/m^3_{soil}$];
- $Z_s$ is the depth of the active surface soil layer [$m_{soil}$]; and
- $\delta_{\text{msw}}$ is a switch which defines the user specified main water feature [-]. Its value is 1 when applied to the main surface water feature and 0 when applied to other surface water features.

5.3.5.5 Cropping

Species are lost from the surface soils due to the cropping cycle. A low rate is conservative for the purpose of assessing consequences of soil exposure. Nutrient cycling in nutrient efficient farms provides a conservative lower bound on the loss of (CSA 2014 recommends 5%) of the nutrient inventory of the crop. The cropping loss $\lambda_{\text{crop}}^j$ for each field type $f$ and species $j$ is defined as (Clause 6.3.7.1 of CSA 2014):

$$\lambda_{\text{crop}}^j(t) = \frac{N_f^j(t) \cdot f_c \cdot \eta_{\text{crop}}^f \cdot \min_{p_{eff}}(\frac{CR_p \cdot Y_p}{h_i})}{Z_s \cdot \rho_{soil}} \quad (5-14)$$
Where,  
\[ \lambda_{\text{crop}}^{j,f}(t) \]  

is the cropping loss rate for each field type \( f \) and species \( j \) [mol/a];  
\[ N_{f}^{j}(t) \]  

is the amount of species \( j \) in surface soil (compartment) \( f \) as determined by AMBER [mol];  

\( f_c \)  

is the fraction of crop elemental composition lost each year [-];  

\( p \in f \) refers to the plants \( p \) that are in field \( f \) (fruits, berries, potatoes and vegetables are in the garden fields, grains and forage crops are in the forage field);  

\[ CR_{p}^{j} \]  

is the plant/soil concentration ratio for species \( j \) and plant \( p \) [kg\(_{\text{soil-dw}}$/kg\(_{\text{plant-fw}}$];  

\( Z_s \)  

is the thickness of the active soil layer [m\(_{\text{soil}}$];  

\( ff_{\text{crop}}^{f} \)  

is the cropping frequency of field \( f \) [a\(^{-1}\)];  

\( \rho_{\text{soil}} \)  

is the soil density [kg\(_{\text{soil-dw}}$/m\(^3\$_{\text{soil}}$]; and  

\( Y_{p} \)  

is the plant yield density for field type \( f \) and plant \( p \) [kg\(_{\text{plant-fw}}$/m\(^2\$_{\text{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).

5.3.5.6 Volatilization

A subset of elements (As, C, Hg, I, S, and Se) are removed from the surface soil via volatilization. Volatilization loss from the soil are modelled assuming transfer rates specified in Table 5-1 from Clause 6.3.5.1 and Clause 6.3.5.2 of CSA (2014). It should be noted that an atmosphere compartment is not defined in the ISM-BIO model. Volatilization losses are removed from the surface soil and transferred to a sink compartment. The air concentration is calculated assuming an equilibrium with the concentration of species in the surface soil (see Section 5.10).

<table>
<thead>
<tr>
<th>Element</th>
<th>( \lambda_{\text{vol}} ) [a(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>( 2.10 \times 10^{-2} )</td>
</tr>
<tr>
<td>S, Se</td>
<td>( 3.20 \times 10^{-2} )</td>
</tr>
<tr>
<td>C</td>
<td>( 1.36 \times 10^{-1} )</td>
</tr>
<tr>
<td>As, Hg, Other</td>
<td>0</td>
</tr>
<tr>
<td>Elements</td>
<td></td>
</tr>
</tbody>
</table>

5.3.5.7 Surface Soil Concentration

The species \( j \) concentration in surface soil for each field type \( f \) [mol/kg\(_{\text{soil}}$] is given by the following equation:

\[
C_{\text{soil}}^{j,f,l}(t) = \frac{N_{f}^{j}(t)}{A^{f} \cdot Z_s \cdot \rho_{\text{soil}}} \quad (5-15)
\]

Where,  
\[ C_{\text{soil}}^{j,f,l}(t) \]  

is the species \( j \) concentration in soil for each field type \( f \) and lifestyle \( l \) [mol/kg\(_{\text{soil}}$];
\( N_j^f(t) \) is the amount of species \( j \) in surface soil (compartment) \( f \) as determined by AMBER [mol];
\( A^f \) is the area of field \( f \) [m\(^2\)soil];
\( Z_s \) is the thickness of the surface soil layer [msoil]; and
\( \rho_{soil} \) is the soil density [kg\(_{dw}\)/m\(^3\)soil].

### 5.4 Surface Water Concentration

Species are discharged from the geosphere to one or more surface water features or topological low points. The ISM-BIO model includes up to three surface water bodies which can represent various surface water features such as rivers, lakes or wetlands. The geosphere outputs determine the amounts discharged to each of these waterbodies (see Section 5.2). The transport processes included in the model are illustrated in Figure 5-6 (adapted from Goodwin et al. 1994).

![Diagram of Surface Water Transport Processes](image)

**Figure 5-6: Surface Water Transport Processes**

### 5.4.1 Surface Water Sources

In addition to ingrowth from radioactive decay, there are four entry routes for radionuclides into the surface water features in the ISM-BIO model. The first is by direct discharge from the aquatic releases from the geosphere. These release rates are calculated by the geosphere model for specific discharge locations (see Section 5.2). The second route of entry is the inflow of contaminated water from other surface water features. The third is through entry from the soil through processes like erosion and leaching. The fourth is from discharge of the domestic water used by the critical group.
5.4.1.1 Aquatic Discharge

The model assumes possible discharge to three different types of surface water bodies (e.g., lakes, rivers or wetlands), in addition to a well discharge. The source flux for each radionuclide to each surface water feature is directly provided by the ISM-GEO model and described in Section 5.2.

5.4.1.2 Flow between Surface Water Features

The rate at which species are transferred from one surface water feature (the “donor” water feature) to another is modelled as follows:

\[ \lambda^{j}_{\text{waterflow}}(t) = \frac{N^{j}_{\text{donor}}(t)Q_{\text{sw}}}{V_{\text{donor}}} \]  

(5-16)

Where,

\( \lambda^{j}_{\text{waterflow}}(t) \) is the rate of transfer rate of species j from the donor surface water feature to the next [mol/a];

\( N^{j}_{\text{donor}}(t) \) is the amount of species j in the donor surface water (compartment) as determined by AMBER [mol];

\( Q_{\text{sw}} \) is the volumetric water flow rate from the donor water feature to the receptor water feature [m³ water/a] or to the sink; and

\( V_{\text{donor}} \) is the volume of the donor water feature [m³ water].

5.4.1.3 Flow from Surface Soil

Influx from the surface soil occurs because of leaching and erosion and are described in Section 5.3.5.3 and Section 5.3.5.4 respectively.

5.4.1.4 Discharge of Domestic Water

All domestic water is conservatively assumed to discharge into the main surface water body. When the well is used, the domestic water becomes a source flux for the main surface water body. The source term is defined as the fraction of the well demand that is used as domestic water. The rate at which species are transferred from domestic water to the main surface water feature is modelled as follows.

\[ \phi^{j,l}_{\text{dom}}(t) = \delta^{j}_{\text{sw}} \cdot X^{j}_{\text{well}}(t) \cdot \frac{f^{l}_{\text{well}} \cdot Q_{\text{dom}}}{Q_{\text{well}}} \]  

(5-17)

Where,

\( \phi^{j,l}_{\text{dom}}(t) \) is the source flux of species j from the well to the main surface water body [mol/a];
δ_{msw} is a switch which defines the user specified main water feature [-]. Its value is 1 when applied to the main surface water feature and 0 when applied to other surface water features; and

\( x_{well}^j(t) \) is the discharge rate of species j from geosphere to the well [mol/a];

\( f_{\text{dom},l}^{\text{well}} \) is the fraction domestic water that is taken from the well (defined in equation (5-18) for lifestyle l;

\( Q_{\text{well}} \) is the total well demand [m\(^3\) \text{water}/a]; and

\( Q_{\text{dom}} \) is the domestic water demand [m\(^3\) \text{water}/a] as defined in Equation (5-23).

\( f_{\text{well}} \) is defined as follows:

For \( l = \text{farmer} \):

\[
 f_{\text{dom},l}^{\text{well}} = \begin{cases} 
 1 & \text{if } Q_{\text{cap}} \geq Q_{\text{dom}} \text{ and well is in use} \\
 Q_{\text{cap}} / Q_{\text{dom}} & \text{if } Q_{\text{cap}} < Q_{\text{dom}} \text{ and well is in use} \\
 0 & \text{if well is not in use or } Q_{\text{cap}} = 0
\end{cases}
\]  

(5-18)

Where,

\( Q_{\text{cap}} \) is the annual well capacity [m\(^3\) \text{water}/a]; and

\( Q_{\text{dom}} \) is the domestic water demand [m\(^3\) \text{water}/a].

For the hunter-gatherer lifestyle (\( l = \text{hunter-gatherer} \)) the well is not used and therefore:

\[
 f_{\text{dom},l}^{\text{well}} = 0
\]  

(5-19)

5.4.2 Surface Water Losses

5.4.2.1 Flow between Surface Water Features

The flow of radionuclides between surface water bodies is described in Section 5.4.1.2 by Equation (5-16).

5.4.2.2 Volatilization

Volatilization losses for surface water bodies are included in the ISM-BIO model. Volatilization loss from the surface waters are modelled assuming transfer rates (\( \lambda_{vol}^{\text{aq}} \)). In general, losses from surface water bodies are expected to be negligible compared to other loss mechanisms, except for C-14 and I-129. C-14 is assumed to have a rate of 2.1 a\(^{-1}\) as specified in clause 6.6.2.5 of CSA (2014) and I-129 is assumed to have a rate of 0.013 a\(^{-1}\) (Connan et al. 2008).

5.4.2.3 Sedimentation

The loss of species from the water column due to sedimentation is described by the sedimentation rate constant (\( \lambda_{\text{sed}}^{\text{sw}} \)). This process is described as a loss from the system (i.e., transfer to the sink), not as a transfer to sediment compartment. Sediment concentrations are
based on the sediment solid-to-liquid partition coefficient ($K_{d_{sed}}^j$). The equation for the sedimentation rate, according to Clause 6.6.2.2 of CSA (2014) is as follows:

$$\lambda_{sed}^j(t) = \frac{N_{sw}^j(t) \cdot DR \cdot \rho_{sed} \cdot A_{sw} \cdot K_{d_{sed}}^j}{V_{sw}}$$

(5-20)

Where,

- $\lambda_{sed}^j(t)$ is the sedimentation rate [mol/a];
- $N_{sw}^j(t)$ is the amount of species $j$ in the surface water (compartment) $sw$ as determined by AMBER [mol];
- DR is the sediment accumulation rate [$m^3_{sediment}/(m^2_{sediment} \cdot a)$];
- $\rho_{sed}$ is the density of sediment [$kg_{sediment-dw}/m^3_{sediment}$];
- $A_{sw}$ is the area of surface water $sw$ sediment [$m^2_{sediment}$];
- $K_{d_{sed}}^j$ is the solid-to-liquid partition coefficient for sediment for species $j$ [$m^3_{water}/kg_{sediment-dw}$]; and
- $V_{sw}$ is the volume of the surface water feature $sw$ [$m^3_{water}$].

### 5.4.3 Surface Water Concentration

The surface water concentration in any surface water feature is calculated as follows:

$$C_{sw}^j(t) = \frac{N_{sw}^j(t) \cdot V_{sw} \cdot \rho}{V_{sw} \cdot \rho}$$

(5-21)

Where,

- $C_{sw}^j(t)$ is concentration of species $j$ in surface water $sw$ [mol/kg$_{water}$];
- $N_{sw}^j$ is the amount of species $j$ in the surface water (compartment) $sw$ as determined by AMBER [mol];
- $V_{sw}$ is the volume of the surface water $sw$ [$m^3_{water}$]; and
- $\rho$ is the density of water [kg/$m^3_{water}$].

In the ISM-BIO the user can specify a main surface water feature. This is the surface water feature used for irrigation of the forage field or to supplement domestic water demands of the critical group if the well is insufficient. The concentration in the main surface water feature is determined by Equation (5-22).

$$C_{msw}^j = \sum_{sw} \delta_{msw} \cdot C_{sw}^j$$

(5-22)

Where,

- $C_{msw}^j$ is concentration of species $j$ in the main surface water [mol/kg$_{water}$];
\( \delta_{msw} \) is a switch which defines the user specified main water feature [-]. Its value is 1 when applied to the main surface water feature and 0 when applied to other surface water features; and

\( C_{sw}^j \) is concentration of species j in surface water sw [mol/kg\text{water}].

### 5.5 Well Water Concentration

The well water may be used as domestic water (for drinking, cooking, bathing, laundering and watering of livestock) and as irrigation water for the garden field for the self-sufficient farmer lifestyle (hunter-gather lifestyle does not use a well for domestic water or irrigation). However, depending on the domestic water needs of the critical group and on the well capacity, these water uses may be partially or fully sourced from the surface water.

The well water concentration depends on the geosphere discharge rate to the well and on the well demand, which in turn depends on the well capacity \( (Q_{cap}) \), the domestic water demand \( (Q_{dom}) \), and the irrigation water demand \( (Q_{irr}) \). These quantities are defined first, before defining the well demand and the well concentration.

The well capacity \( (Q_{cap}) \) is the annual capacity of the well to supply water \([m^3/a]\). Its value is not calculated, but rather input by the user as a feature of the biosphere.

The domestic water demand is defined as follows:

\[
Q_{dom} = N_{crit} \cdot Q_{pc} + \sum_{ls} \left( N_{ls} \cdot \frac{R_{ing,ls} \cdot \rho_{wat}}{\rho_{wat}} \right)
\]  

(5-23)

Where,

- \( Q_{dom} \) is the domestic water demand \([m^3_{\text{water}}/a]\);
- \( N_{crit} \) is the number of people in the critical group [-];
- \( Q_{pc} \) is the annual adult water demand per person for drinking and domestic use \([m^3_{\text{water}}/ (\text{person-a})]\);
- \( N_{ls} \) is the number of livestock \( \text{ls} \) [-] defined in Equation (5-4);
- \( R_{ing,ls} \) is the livestock \( \text{ls} \) ingestion rate of water \([\text{kg}_{water}/a]\); and
- \( \rho_{wat} \) is the density of water \([\text{kg}_{water}/m^3_{\text{water}}]\).

The annual irrigation water demand for watering the garden \( (Q_{irr}) \) is defined as:

\[
Q_{irr} = R_{irr}^f \cdot A^f \text{ for } f = \text{garden}
\]  

(5-24)

Where,

- \( Q_{irr} \) is the irrigation water demand \([m^3_{\text{water}}/a]\);
- \( R_{irr}^f \) is the irrigation rate of field \( f \) \([m^3_{\text{water}}/ (m^2_{\text{soil}} \text{a})]\); and
- \( A^f \) is the area of field \( f \) \([m^2_{\text{soil}}]\).

The total well demand depends on the domestic water demand, the irrigation water demand and the well capacity.
If the well capacity can meet the domestic water needs (i.e., drinking, bathing, watering of livestock) and also irrigate the garden is also irrigated using well water (i.e., $Q_{\text{cap}} \geq Q_{\text{dom}} + Q_{\text{irr}}$), then the well annual flow is:

$$Q_{\text{well}} = Q_{\text{dom}} + Q_{\text{irr}} \quad (5-25)$$

Where,

- $Q_{\text{well}}$ is the total well demand [m$^3$/water/a],
- $Q_{\text{dom}}$ is the domestic water demand [m$^3$/water/a],
- $Q_{\text{irr}}$ is the irrigation water demand [m$^3$/water/a]; and
- $Q_{\text{cap}}$ is the capacity of the well to provide water [m$^3$/water/a].

If the well is the primary water source, but it cannot cover all domestic and garden irrigation needs (i.e., $Q_{\text{cap}} < Q_{\text{dom}} + Q_{\text{irr}}$) then the well annual flow is limited to its capacity:

$$Q_{\text{well}} = Q_{\text{cap}} \quad (5-26)$$

Finally, the well concentration [mol/kg] is described as follows:

$$C^j_{\text{well}} = \frac{X^j_{\text{well}} \cdot \delta_{\text{well}}}{Q_{\text{well}} \cdot \rho_{\text{wat}}} \quad (5-27)$$

Where,

- $C^j_{\text{well}}$ is the concentration of species $j$ in the well [mol/kg];
- $X^j_{\text{well}}$ is the discharge rate from geosphere to the well for species $j$ [mol/a];
- $Q_{\text{well}}$ is the total well demand [m$^3$/water/a];
- $\rho_{\text{wat}}$ is the water density [kg/m$^3$/water]; and
- $\delta_{\text{well}}$ is a switch that determines the well's usage (use of well=1, no well=1).

### 5.6 Groundwater Concentration

In reality, 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:

$$C^j_{\text{groundwater}} = C^j_{\text{well}} \quad (5-28)$$

The groundwater concentration is only used for comparison with chemically hazardous species acceptance criteria.
5.7 Domestic Water Concentration

The domestic water is the water used by the critical group for drinking, bathing, laundry, and watering of animals. Depending on the well capacity, the domestic water needs and the lifestyle, the domestic water concentration can refer to the well concentration, the surface water concentration or a combination of both.

The domestic water supply for the hunter-gatherer is always assumed to be the main surface water feature. Therefore, for the hunter-gatherer (l= hunter-gatherer):

\[ C_{dom}^{j, hunter-gatherer} = c_{msw}^{j} \] (5-29)

Where,

- \( c_{msw}^{j} \) is the concentration of species \( j \) in the main surface water feature [mol/kgwater].

For the farmer (l= farmer), the domestic water concentration is described by Equation (5-30).

\[ C_{dom}^{j, farmer} = f_{well}^{dom} c_{well}^{j} + f_{sw}^{dom} c_{msw}^{j} \] (5-30)

Where,

- \( c_{well}^{j} \) is the concentration of species \( j \) in the well [mol/kgwater];
- \( f_{well}^{dom} \) is the fraction of domestic water that is sourced from the well [-] defined in Equation (5-18); and
- \( f_{sw}^{dom} \) is the fraction of domestic water that is sourced from the surface water for the farmer \((1-f_{well}^{dom})\).

5.8 Irrigation Water Concentration

The farmer’s garden field is assumed to be irrigated with water that is sourced from either the well or the main surface water feature, depending on the well demand. The forage field is assumed to be irrigated with surface water for the farming lifestyle. The hunter-gatherer is not assumed to irrigate fields.

As with the domestic water concentration, the fraction of well water and surface water that is used for irrigation depends on the well capacity \((Q_{cap})\), the domestic water demand \((Q_{dom})\) and the irrigation water needs \((Q_{irr})\). For the farming lifestyle, well water is used preferentially for domestic water needs; the garden is irrigated with well water only if the well capacity meets the domestic and irrigation water needs. Therefore, in the farming lifestyle the garden irrigation water concentration is expressed as follows:
\[ C_{\text{irr}}^{j,f,l} = f_{\text{well}}^{\text{irr},f,l} \cdot C_{\text{well}}^{j,l} + f_{\text{sw}}^{\text{irr},f,l} \cdot C_{\text{msw}}^{j,l} \text{ for } l = \text{farmer and } f = \text{garden} \] (5-31)

Where,
- \( C_{\text{irr}}^{j,f,l} \) is the concentration of species \( j \) in the irrigation water \([\text{mol/m}^3\text{water}]\);
- \( f_{\text{well}}^{\text{irr},f,l} \) is the fraction of irrigation water that is sourced from well (see Section 5.3.5.1);
- \( f_{\text{sw}}^{\text{irr},f,l} \) is the fraction of irrigation water that is sourced from surface water (see Section 5.3.5.2);
- \( C_{\text{well}}^{j,l} \) is the concentration of species \( j \) in the well water \([\text{mol/m}^3\text{water}]\); and
- \( C_{\text{msw}}^{j,l} \) is the main surface water concentration of species \( j \) \([\text{mol/m}^3\text{water}]\).

For the farmer’s forage field, the irrigation is assumed to be taken from the main surface water feature, and therefore:

\[ C_{\text{irr}}^{j,f,l} = C_{\text{msw}}^{j,l} \text{ for } l = \text{farmer and } f = \text{forage} \] (5-32)

The hunter-gatherer is not assumed to irrigate fields, and therefore:

\[ C_{\text{irr}}^{j,f,l} = 0 \text{ for } l = \text{hunter - gatherer and } f = \text{forage/garden} \] (5-33)

### 5.9 Sediment Concentration

According to Clause 7.8.1 of CSA (2014), radionuclides are assumed to be deposited to beach sediment by wave action. Thus, the concentration in beach sediment is described with the following equation:

\[ C_{\text{sed}}^{j} = C_{\text{msw}}^{j} \cdot p_{\text{wat}}^{\text{sed}j} \] (5-34)

Where,
- \( C_{\text{msw}}^{j} \) is the concentration of species \( j \) in the sediment \([\text{mol/kgsediment-dw}]\);
- \( C_{\text{msw}}^{j} \) is the concentration of species \( j \) in the main surface water feature \([\text{mol/kgwater}]\); and
- \( p_{\text{wat}}^{\text{sed}j} \) is the transfer of dissolved species \( j \) in beach sediment \([\text{kgwater/kgsediment-dw}]\).

Default values for \( p_{\text{wat}}^{\text{sed}j} \) are listed in Table A.26 of CSA (2014).
5.10 Atmosphere Concentration

CSA (2014) provides guidance on modelling airborne concentration from effluent releases from facilities. However, because of the nature of the releases from a repository, many of the equations describing atmosphere concentration do not apply to this model.

As per the CSA (2014), the atmosphere concentration is modelled as an equilibrium process. In general, species can enter the atmosphere from soils and surface waters via volatilization. In the ISM-BIO model, the atmosphere concentration used to calculate exposures to human and non-human biota, is assumed to be the atmosphere above the most contaminated field.

Implicit in this approach is the assumption that the atmosphere above the fields and surface waters do not mix. In addition members of the critical group are assumed to spend all of their time in the atmosphere above the most contaminated field.

For volatile species, the equilibrium factor describing the concentration in air from volatilization from soil is as follows (Clause 7.2.5.1 of CSA 2014):

\[
P_{\text{soil}}^{\text{air}} = Z_{\text{soil}} \cdot \rho_{\text{soil}} \cdot \lambda_{\text{vol}} \cdot D_{\text{res}} \cdot C_{\text{res}} \tag{5-35}\]

Where,

- \(P_{\text{soil}}^{\text{air}}\) is the transfer parameter from irrigated soil to air for species \(j\) [kg_{soil-dw}/m^3_{air}];
- \(Z_{\text{soil}}\) is the depth of the surface soil [m_{soil}];
- \(\rho_{\text{soil}}\) is the soil density [kg_{soil-dw}/m^3_{soil}];
- \(\lambda_{\text{vol}}\) is the terrestrial volatilization rate constant for species \(j\) [a^{-1}];
- \(D_{\text{res}}\) is the air dilution factor for terrestrial volatilization [a m^2_{soil}/m^3_{air}]; and
- \(C_{\text{res}}\) is a correction factor that accounts for the location of the receptor relative to the field [-]. This is assumed to be 1 in the ISM-BIO model but a more complex relationship can be defined (e.g., clause 7.2.5.3 of CSA 2014).

The air dilution factor for terrestrial volatilization [a/m] accounts for dispersion in air from the source to the receptor. It is given by (CSA 2014):

\[
D_{\text{res}} = (4.87A_f^{\frac{1}{6}} - 3.56) \cdot f_{s-a} \tag{5-36}\]

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

The air concentration for a receptor near a field is expressed as follows:

\[
C_{\text{air}}^{j} = \max \left\{ P_{\text{soil}_{\text{garden}}}^{\text{air}} \cdot C_{\text{soil}_{\text{garden}}}^{j}, P_{\text{soil}_{\text{forage}}}^{\text{air}} \cdot C_{\text{soil}_{\text{forage}}}^{j} \right\} \tag{5-37}\]
5.11 Concentration in Plants and Animals

The concentration in plants and animals (livestock and wildlife) is calculated based on the concentrations in environmental media that were calculated using the methodologies in Sections 5.4 to 5.10. Figure 5-2 illustrates the pathways that lead to contamination of plant and animal tissues.

The concentration in plants and animals depends on the following concentrations:

\[ C_{\text{soil}}^i \] is the concentration of radionuclide i in the soil of field f for lifestyle l [Bq/kg_{soil-dw}];

\[ C_{\text{msw}}^i \] is the concentration of radionuclide i in the main surface water feature [Bq/kg_{water}];

\[ C_{\text{well}}^i \] is the concentration of radionuclide i in the well [Bq/kg_{water}];

\[ C_{\text{sed}}^i \] is the concentration of radionuclide i in sediment [Bq/kg_{sediment-dw}]; and

\[ C_{\text{air}}^i \] is the air concentration of radionuclide i and lifestyle l [Bq/m^3_{air}].

Species concentrations, as derived in Sections 5.3.5.7, 5.4.3, 5.5, 5.6, 5.9 and 5.10 above, are converted to radionuclide concentrations using molar mass and indexed over radionuclides (thus dropping the stable elements for dose calculations). Note that, conservatively, the amount of nuclide in a given media is not reduced by the transfer of some nuclide into plants or animals.

5.11.1 Plants

Plants are assumed to be consumed by humans and animals. The model considers five types of plants as listed in CSA (2014). Each of these plant types are assumed to be grown in a particular field type. These are shown in Table 5-2.

<table>
<thead>
<tr>
<th>Field Type</th>
<th>Plant Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Garden</td>
<td>Fruits and berries</td>
</tr>
<tr>
<td></td>
<td>Vegetables</td>
</tr>
<tr>
<td></td>
<td>Potatoes</td>
</tr>
<tr>
<td>Forage</td>
<td>Forage feed</td>
</tr>
<tr>
<td></td>
<td>Grain (for human consumption)</td>
</tr>
</tbody>
</table>

For each plant p, the concentration of radionuclide i is given by the following equation:

\[ C_{p}^i = C_{\text{irr}}^i \cdot P_{\text{irr}}^p + C_{\text{soil}}^i \cdot P_{\text{soil}}^p + C_{\text{air}}^i \cdot P_{\text{air}}^p \]  \( (5-38) \)

Where,

\[ C_{p}^i \] is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg_{plant-fw}];

\[ C_{\text{irr}}^i \] is the concentration of radionuclide i in irrigation water for lifestyle l [Bq/kg_{water}];

\[ C_{\text{soil}}^i \] is the concentration of radionuclide i in soil f that contains plant p for lifestyle l [Bq/kg_{soil-dw}];

\[ C_{\text{air}}^i \] is the air concentration of radionuclide i [Bq/m^3_{air}];
\( p_{\text{irr}}^{i,p} \) is the transfer parameter for the irrigation water concentration to the plant concentration for radionuclide \( i \) [\( \text{kg}_{\text{water}}/\text{kg}_{\text{plant-fw}} \)];

\( p_{\text{soil}}^{i,p} \) is the transfer parameter for soil concentration to plant concentration for radionuclide \( i \) [\( \text{kg}_{\text{soil-dw}}/\text{kg}_{\text{plant-fw}} \)]; and

\( p_{\text{air}}^{i,p} \) is the transfer parameter for air concentration to plant concentration for radionuclide \( i \) [\( \text{m}^3_{\text{air}}/\text{kg}_{\text{plant-fw}} \)].

The transfer from water to plants occurs as a result of irrigation of plants. Every time plants are irrigated, it is assumed that the plant retains a volume of water that is proportional to the leaf area. The transfer parameter for irrigation water to plants (\( p_{\text{irr}}^{i,p} \)) is given by the following equation (Equation 7-13 from Clause 7.3.1.1 of CSA 2014):

\[
p_{\text{irr}}^{i,p} = \frac{\text{LAI} \cdot I_{\text{wt}} \cdot \eta_{\text{I}} \cdot t_{\text{f}} \cdot h_{\text{i}} \cdot \left[ 1 - e^{-\lambda_{e,i}^{\text{p},\text{wet}}} \right]}{\lambda_{e}^{\text{p}} \cdot Y_{\text{p}}} \tag{5-39}
\]

Where,

\( p_{\text{irr}}^{i,p} \) is the transfer parameter for the irrigation water concentration to the plant concentration [\( \text{kg}_{\text{water}}/\text{kg}_{\text{plant-fw}} \)];

\( \text{LAI} \) is the leaf area index (leaf area per unit surface area) [\( \text{m}^2_{\text{leaf}}/\text{m}^2_{\text{soil}} \)];

\( I_{\text{wt}} \) is the mass of water retained per unit leaf area [\( \text{kg}_{\text{water}}/\text{m}^2_{\text{leaf}} \)];

\( \eta_{\text{I}} \) is the frequency of irrigation events per year [\( \text{a}^{-1} \)];

\( t_{\text{f}} \) is the translocation factor from foliage to consumable product [-];

\( h_{\text{i}} \) is the harvest index (mass of consumable product divided by mass of total above-ground plant [-]);

\( \lambda_{e}^{\text{p}} \) is the effective removal constant from vegetation surfaces for radionuclide \( i \) and plant \( p \) [\( \text{a}^{-1} \)];

\( Y_{\text{p}} \) is the plant yield density for plant \( p \) [\( \text{kg}_{\text{plant-fw}}/\text{m}^2_{\text{soil}} \)]; and

\( t_{\text{wet}}^{\text{p}} \) is the effective duration of the wet deposition [\( \text{a} \)].

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:

\[
\lambda_{e}^{\text{p}} = \lambda_{\text{i}} + \lambda_{\text{veg}}^{\text{p}} \tag{5-40}
\]

Where,

\( \lambda_{\text{i}} \) is the effective removal constant from vegetation surfaces for radionuclide \( i \) and plant \( p \) [\( \text{a}^{-1} \)];

\( \lambda_{\text{i}}^{\text{p}} \) is the radioactive decay constant [\( \text{a}^{-1} \)]; and

\( \lambda_{\text{veg}}^{\text{p}} \) is the removal constant from vegetation surfaces for plant \( p \) [\( \text{a}^{-1} \)].

Radionuclides are transferred from the soil to plants through uptake by the roots. The transfer parameter that describes this process (\( p_{\text{soil}}^{i,p} \)) is given by the following equation (Equation 6-62 from Clause 6.8.1 of CSA 2014):
Where,

\[ p_{soil}^{i,p} \] is the transfer parameter for soil concentration to plant concentration for radionuclide \( i \) \([\text{kg}_{\text{soil-dw}}/\text{kg}_{\text{plant-fw}}]\); and

\[ CR_p^i \] is the plant/soil concentration ratio of radionuclide \( i \) for plant \( p \) \([\text{kg}_{\text{soil-dw}}/\text{kg}_{\text{plant-fw}}]\).

The concentration ratio is often expressed on a plant dry weight basis, instead of a fresh weight basis, as is done in Equation (5-41). If this is the case, the concentration ratio should be divided by \( DW_p \), the dry/fresh weight ratio for plants.

Radionuclides are transferred from air to plants through dry deposition. The transfer parameter that describes this process \( (P_{air}^{i,p}) \) is given by the following equation (Equation 6-35 from Clause 6.4.1 of CSA (2014))

\[
P_{air}^{i,p} = \frac{v_g^i \cdot f_{int} \cdot t_f \cdot h_i \cdot [1 - e^{-\lambda e t_{efr}^i}]}{\lambda e \cdot Y_p}
\] (5-42)

Where,

\[ p_{air}^{i,p} \] is the transfer parameter for air concentration to plant concentration for radionuclide \( i \) \([\text{m}^3/\text{kg}_{\text{plant-fw}}]\);

\[ v_g^i \] is the deposition velocity of radionuclide \( i \) \([\text{m}/\text{a}]\);

\[ f_{int} \] is the foliar intersection fraction \([-]\);

\[ t_{efr}^i \] is the effective duration of the dry deposition \([\text{a}]\); and

\( t_f, h_i, \lambda e, Y_p \) are as defined in Equation (5-39).

According to Equation 6-31a from Clause 6.3.3.1 of CSA (2014), the deposition velocity is a combination of the dry deposition velocity \( (v_d^i, \text{m}/\text{y}) \) and the wet deposition velocity \( (v_w^i, \text{m}/\text{y}) \), as follows:

\[ v_g^i = v_d^i + v_w^i \] (5-43)

Where,

\[ v_g^i \] is the deposition velocity \([\text{m}_{\text{soil}}/\text{a}]\);

\[ v_d^i \] is the dry deposition velocity \([\text{m}_{\text{soil}}/\text{a}]\); and

\[ v_w^i \] is the wet deposition velocity \([\text{m}_{\text{soil}}/\text{a}]\).

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 (2014)):

\[ v_w^i = W_r \cdot P_{tot} \] (5-44)

Where,
\( W_r \) is the washout ratio [-]; and
\( P_{tot} \) is the annual precipitation rate [m\text{soil}/a].

### 5.11.2 Animals

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

**Table 5-3: Animal Groupings**

<table>
<thead>
<tr>
<th>Animal Group</th>
<th>Animals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Livestock</td>
<td>Dairy Cattle, Beef Cattle, Pig, Lamb, Goat, Chicken</td>
</tr>
<tr>
<td>Aquatic Wildlife</td>
<td>Aquatic plants*, Fish</td>
</tr>
<tr>
<td>Terrestrial Wildlife</td>
<td>Deer, Rabbit, Duck, Muskrat</td>
</tr>
</tbody>
</table>

*Even though Aquatic Plants are not animals, they are considered here because the method to calculate the concentration is the same as that for the Fish.*

#### 5.11.2.1 Livestock

The concentration of radionuclide \( i \) in livestock tissue is given by the following equation:

\[
C_{ls}^{i,l} = C_{air}^{i,l} \cdot P_{air}^{i,ls} + C_p^{i,l} \cdot P_p^{i,ls} + C_{soil}^{i,f} \cdot P_{soil}^{i,ls} + C_{dom}^{i,l} \cdot P_{dom}^{i,ls}
\]

for \( f = \text{forage} \) and \( p = \text{forage feed} \)

Where,
- \( C_{ls}^{i,l} \) is the concentration of radionuclide \( i \) in livestock for lifestyle \( l \) [Bq/kg\text{livestock-fw}];
- \( C_{air}^{i,l} \) is the air concentration of radionuclide \( i \) and lifestyle \( l \) [Bq/m\text{3}];
- \( C_p^{i,l} \) is the concentration of radionuclide \( i \) in plant for lifestyle \( l \) [Bq/kg\text{livestock-dw}];
- \( C_{soil}^{i,f} \) is the concentration of radionuclide \( i \) in the soil of field \( f \) and lifestyle \( l \) [Bq/kg\text{soil-dw}];
- \( C_{dom}^{i,l} \) is the concentration of radionuclide \( i \) in domestic water for lifestyle \( l \) [Bq/kg\text{water}];
- \( P_{air}^{i,ls} \) is the transfer parameter for air concentration to livestock \( ls \) tissue concentration for radionuclide \( i \) [m\text{3}/kg\text{livestock-fw}];
- \( P_p^{i,ls} \) is the transfer parameter for plant concentration to livestock \( ls \) tissue concentration for radionuclide \( i \) [kg\text{plant-dw}/kg\text{livestock-dw}];
- \( P_{soil}^{i,ls} \) is the transfer parameter for soil concentration to livestock \( ls \) tissue concentration for radionuclide \( i \) [kg\text{soil-dw}/kg\text{livestock-fw}]; and
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 2014):

$$p_{\text{air}, \text{ls}} = R_{\text{inh}} \cdot f_{\text{inh}}^{\text{ls}}$$  \hspace{1cm} (5-46)$$

Where,

- $p_{\text{air}, \text{ls}}$ is the transfer parameter for air concentration to livestock ls tissue concentration for radionuclide i [m$^3$/kg$\text{air}$/kg$\text{livestock-fw}$];
- $R_{\text{inh}}$ is the livestock inhalation rate [m$^3$/a]; and
- $f_{\text{inh}}^{\text{ls}}$ 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 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 2014):

$$p_{\text{p}, \text{ls}} = \frac{r_{\text{feed}}^{\text{ls}} \cdot R_{\text{ing,feed}} \cdot f_{\text{ing}}^{\text{ls}} \cdot e^{-\lambda_i t_h}}{DW_p}$$  \hspace{1cm} (5-47)$$

Where,

- $p_{\text{p}, \text{ls}}$ is the transfer parameter for plant concentration to livestock ls tissue concentration for radionuclide i [kg$\text{plant-dw}$/kg$\text{plant-dw}$];
- $r_{\text{feed}}^{\text{ls}}$ is the fraction of feed from contaminated sources [-];
- $R_{\text{ing,feed}}$ is the livestock ls ingestion rate of feed [kg$\text{plant-dw}$/a];
- $f_{\text{ing}}^{\text{ls}}$ is the fraction of the livestock’s annual intake by ingestion that appears in each kg of livestock [a/kg$\text{livestock-fw}$];
- $\lambda_i$ is the radioactive decay constant of radionuclide i [a$^{-1}$];
- $t_h$ 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 [kg$\text{plant-dw}$/kg$\text{plant-dw}$].

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 2014):

$$p_{\text{soil}, \text{ls}} = \left( f_{\text{cont}}^{\text{feed}} \cdot R_{\text{ing,feed}}^{\text{ls}} \cdot f_{\text{sl}} + R_{\text{ing,soil}}^{\text{ls}} \right) \cdot f_{\text{ing}}^{\text{ls}}$$  \hspace{1cm} (5-48)$$

Where,

- $p_{\text{soil}, \text{ls}}$ is the transfer parameter for soil concentration to livestock ls tissue concentration for radionuclide i [kg$\text{soil-dw}$/kg$\text{livestock-fw}$];
- $f_{\text{cont}}^{\text{feed}}$ is the fraction of feed from contaminated sources [-]; and
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 2014):

\[
P_{\text{dom}}^{\text{ils}} = f_w \cdot R_{\text{ing, wat}}^{\text{ils}} \cdot F_{\text{ing}}^{\text{ils}}
\]  
(5-49)

Where,

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

Note that CSA (2014) treats C-14 differently for the transfer to livestock. However, the intricacies of the C-14 behaviour are not modelled in the biosphere model.

5.11.2.2 Aquatic Biota

The aquatic biota considered in the 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:

\[
C_{\text{ab}} = C_{\text{msw}} \cdot p_{\text{msw}}^{\text{lab}}
\]  
(5-50)

Where,

- \( C_{\text{ab}} \) is the concentration of radionuclide i in the aquatic biota [Bq/kg\text{ab-fw}];
- \( C_{\text{msw}} \) is the concentration of radionuclide i in the main surface water feature [Bq/kg\text{water}]; and
- \( p_{\text{msw}}^{\text{lab}} \) is the transfer parameter for the main surface water feature concentration to aquatic biota tissue concentration for radionuclide i [kg\text{water/kg ab-fw}].

The transfer parameter for water to aquatic biota is described by the bioaccumulation factor (BAF_{\text{msw}}^{\text{ab}}[\text{kg\text{water/kg ab-fw}}]) for each aquatic biota and radionuclide i (Equation 7-20 from Clause 7.7.1 of CSA 2014):

\[
p_{\text{msw}}^{\text{lab}} = \text{BAF}_{\text{ab}}
\]  
(5-51)
5.11.2.3 Wildlife

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

\[
C_{wl}^{i,l} = C_{air}^{i,l} \cdot P_{air}^{i,l} + C_{p}^{i,l} \cdot P_{p}^{i,l} + C_{ab}^{i} \cdot P_{ab}^{i,l} + C_{soil}^{i,l} \cdot P_{soil}^{i,l} + C_{msw}^{i} \cdot P_{msw}^{i,l}
\]

(5-52)

Where,

\(C_{wl}^{i,l}\) is the concentration of radionuclide \(i\) in the wildlife sl for lifestyle \(l\) [Bq/kg wildlife-fw];

\(P_{air}^{i,l}\) is the transfer parameter for air concentration to wildlife \(wl\) tissue concentration for radionuclide \(i\) [m\(^3\)/kg wildlife-fw];

\(P_{p}^{i,l}\) is the transfer parameter for plant \(p\) concentration to wildlife \(wl\) tissue concentration for radionuclide \(i\) [-];

\(P_{ab}^{i,l}\) is the transfer parameter for aquatic biota to wildlife tissue [-];

\(P_{soil}^{i,l}\) is the transfer parameter from soil concentration to wildlife tissue concentration for radionuclide \(i\) [kg soil-dw/kg wildlife-fw];

\(P_{msw}^{i,l}\) is the transfer parameter for the main surface water concentration to wildlife \(wl\) tissue concentration for radionuclide \(i\) [kg water/kg wildlife-fw]; and \(C_{air}^{i,l}, C_{p}^{i,l}, C_{ab}^{i}, C_{soil}^{i}, C_{msw}\) are as defined above.

The transfers from air, soil and water are similar as those described in Equations (5-46) to (5-49) respectively, except that the \(ls\) (livestock) is replaced by \(wl\) (wildlife). The transfer to wildlife from plants is similar to equation (5-47), except that because wildlife eats directly from the field, the exponential term disappears. The transfer to wildlife from the consumption of aquatic biota \(P_{ab}^{wl,i}\) is described as follows (derived from Equation 6-68 of CSA 2014):

\[
P_{ab}^{wl,i} = r_{feed} \cdot R_{ing,ab}^{wl} \cdot F_{ing}^{i, wl} \cdot f_{ing,ab}^{wl} / DW_{ab}
\]

(5-53)

Where,

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

\(r_{feed}\) is the fraction of feed from contaminated sources [-];

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

\(F_{ing}^{i, wl}\) is the fraction of the wildlife’s annual intake by ingestion that appears in each kg of produce [a/kg ab-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-dw/kg ab-fw].
5.12 Human Dose Pathways

Doses to humans are calculated for the following pathways illustrated in Figure 5-3. All dose rates are indexed over three different age groups (adult, child and infant) and the two different lifestyles (farmer and hunter-gatherer). The user selects the age group and the lifestyle to be modelled.

5.12.1 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:

\[ D_{ing}^{i, a, l} = \sum_{p} p_{ing,p}^{i, a, l} \cdot C_{p}^{i, l} + \sum_{WL} p_{ing, WL}^{i, a, l} \cdot C_{WL}^{i, l} + \sum_{ls} p_{ing, ls}^{i, a, l} \cdot C_{ls}^{i, l} + \sum_{ab} p_{ing, ab}^{i, a, l} \cdot C_{ab}^{i, l} + p_{ing, wat}^{i, a, l} \cdot C_{dom}^{i, l} \]

\[ + p_{ing, soil}^{i, a, l} \cdot \max \left( \frac{C_{i, garden}^{i.sourceforge, l}}{C_{soil}^{i, l}}, \frac{C_{i, forage, l}}{C_{soil}^{i, l}} \right) + p_{ing, sed}^{i, a, l} C_{sed}^{i, l} \]

for \( f = \text{garden} \)

Where,

- \( D_{ing}^{i, a, l} \) is the human dose rate through ingestion for radionuclide i, age group a and lifestyle l [Sv/a];
- \( p_{ing,p}^{i, a, l} \) 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})];
- \( p_{ing, WL}^{i, a, l} \) 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})];
- \( p_{ing, ls}^{i, a, l} \) 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})];
- \( p_{ing, ab}^{i, a, l} \) 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})];
- \( p_{ing, wat}^{i, a, l} \) 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})];
- \( p_{ing, soil}^{i, a, l} \) 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\text{soil-dw})];
- \( p_{ing, sed}^{i, a, l} \) 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\text{sediment-dw})];
- \( C_{p}^{i, l} \) is the concentration of radionuclide i in plant p for lifestyle l [Bq/kg\text{plant-fw}];
- \( C_{WL}^{i, l} \) is the concentration of radionuclide i in livestock ls for lifestyle l [Bq/kg\text{livestock-fw}];
- \( C_{ls}^{i, l} \) is the concentration of radionuclide i in wildlife wl for lifestyle l [Bq/kg\text{wildlife-fw}];
- \( C_{ab}^{i, l} \) is the concentration of radionuclide i in aquatic biota ab [Bq/kg\text{ab-fw}];
- \( C_{dom}^{i, l} \) is the concentration of radionuclide i in domestic water for lifestyle l [Bq/kg\text{water}];
5.12.1.1 Food

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

$$P_{ing,y}^{i,al} = f_y \cdot f_{cont}^{y} \cdot R_{ing,y}^{al} \cdot DCF_{ing}^{i,a}$$ (5-55)

Where,

- $P_{ing,y}^{i,al}$ 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 food-fw)];
- $f_y$ is the adjustment factor for processing food j [-];
- $f_{cont}^{y}$ is the fraction from contaminated sources of food type j [-];
- $R_{ing,y}^{al}$ is the ingestion rate of food type j for lifestyle l and age group a [kg food-fw/a];
- DCF_{ing}^{i,a} 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).

5.12.1.2 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 2014):

$$P_{ing,wat}^{i,al} = f_w \cdot R_{ing,wat}^{al} \cdot DCF_{ing}^{i}$$ (5-56)

Where,

- $P_{ing,wat}^{i,al}$ 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 water)];
- $f_w$ is the fraction of drinking water from contaminated sources [-];
- $R_{ing,wat}^{al}$ is the ingestion rate of water for lifestyle l and age group a [kg water/a]; and
- DCF_{ing}^{i,a} is the dose conversion factor for radionuclide i for intake by ingestion for age group a [Sv/Bq].

5.12.1.3 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 2014):
\[ p_{\text{soil,ing}}^{i,a,l} = R_{\text{ing,soil}}^{i,a,l} \cdot f_{\text{soil}} \cdot DCF_{\text{ing}}^{i,a} \] (5-57)

Where,

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

### 5.12.1.4 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 2014):

\[ p_{\text{sed,ing}}^{i,a,l} = R_{\text{ing,sed}}^{i,a,l} \cdot f_{\text{sed}} \cdot DCF_{\text{ing}}^{i,a} \] (5-58)

Where,

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

### 5.12.2 Inhalation Dose Rates

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

\[ D_{\text{inh}}^{i,a,l} = p_{\text{inh}}^{i,a,l} \cdot C_{\text{air}}^{i,l} \] (5-59)

Where,

- \( D_{\text{inh}}^{i,a,l} \): human dose rate through ingestion for radionuclide \( i \), age group \( a \) and lifestyle \( l \) \([\text{Sv}/\text{a}]\);
- \( p_{\text{inh}}^{i,a,l} \): transfer parameter for outdoor air concentration to dose rate from inhalation for radionuclide \( i \), age group \( a \) and lifestyle \( l \) \([\text{Sv}/\text{a}] \cdot (\text{Bq}^2/\text{m}^3_{\text{air}})^{-1}\); and
- \( C_{\text{air}}^{i,l} \): outdoor air concentration of radionuclide \( i \) for lifestyle \( l \) \([\text{Bq}/\text{m}^3_{\text{air}}]\).

The transfer parameter from outdoor air to dose rate from inhalation is defined as follows (Equation 6-79 from Clause 6.13.1 of CSA 2014):
\[ p_{\text{inh}}^{i,a,l} = R_{\text{inh}}^a \cdot \text{OF}_{\text{area}} \cdot \text{DCF}_{\text{inh}}^{i,a} \] (5-60)

Where,

- \( p_{\text{inh}}^{i,a,l} \) is the transfer parameter for outdoor air concentration to dose rate from inhalation for radionuclide \( i \), age group \( a \), and lifestyle \( l \) \([\text{(Sv/a)/(Bq/m}^3_{\text{air}})]\);
- \( R_{\text{inh}}^a \) is the human’s inhalation rate for age group \( a \) \([\text{m}^3_{\text{air}}/\text{a}]\);
- \( \text{OF}_{\text{area}} \) is the area occupancy factor [-]; and
- \( \text{DCF}_{\text{inh}}^{i,a} \) is the dose conversion coefficient for intake by inhalation for radionuclide \( i \) for age group \( a \) \([\text{(Sv)/(Bq)}] \).

5.12.3 External Dose Rates

The critical group is externally exposed to species in soil and in sediment along the beaches as well as externally exposed by immersion in air and water. These three routes of exposure are detailed here.

5.12.3.1 Air Immersion Rates

The air immersion dose rates are the sum of the effective whole-body dose and the skin dose, and the sum of indoor and outdoor exposures. It is expressed as follows:

\[ D_{\text{imm,air}}^{i,a,l} = p_{\text{imm}}^{i,a,l} \cdot C_{\text{air}}^{i,l} \] (5-61)

Where,

- \( D_{\text{imm,air}}^{i,a,l} \) is the human dose rate through air immersion for radionuclide \( i \), age group \( a \) and lifestyle \( l \) \([\text{Sv/a}]\);
- \( p_{\text{imm}}^{i,a,l} \) is the transfer parameter for outdoor air concentration to total rate dose from immersion for radionuclide \( i \) for age group \( a \) and lifestyle \( l \) \([\text{(Sv/a)/(Bq/m}^3_{\text{air}})]\); and
- \( C_{\text{air}}^{i,l} \) is the outdoor air concentration of radionuclide \( i \) lifestyle \( l \) \([\text{Bq/m}^3_{\text{air}}]\).

The transfer parameter from outdoor air concentration to the dose rate from immersion in air is calculated as follows:

\[ p_{\text{imm}}^{i,a,l} = \text{OF}_{\text{area}} \cdot \text{DCF}_{\text{imm,air}}^{i,a} \] (5-62)

Where,

- \( p_{\text{imm}}^{i,a,l} \) is the transfer parameter for outdoor air concentration to total rate dose from immersion for radionuclide \( i \) for age group \( a \) and lifestyle \( l \) \([\text{(Sv/a)/(Bq/m}^3_{\text{air}})]\);
- \( \text{OF}_{\text{area}} \) is the area occupancy factor [-]; and
- \( \text{DCF}_{\text{imm,air}}^{i,a} \) is the effective dose conversion coefficient for a semi-infinite cloud for radionuclide \( i \) for age group \( a \) \([\text{(Sv)/(Bq/m}^3_{\text{air}})]\).
5.12.3.2 Water Immersion Dose Rates

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

\[
D_{imm,\text{wat}}^{i,a,l} = P_{imm,\text{dom}}^{i,a,l} \cdot C_{\text{dom}}^{i,l} + P_{imm,\text{msw}}^{i,a,l} \cdot C_{\text{msw}}^{i,l} \tag{5-63}
\]

Where,

- \(D_{imm,\text{wat}}^{i,a,l}\) is the human dose rate through water immersion for radionuclide \(i\), age group \(a\) and lifestyle \(l\) [Sv/a];
- \(P_{imm,\text{dom}}^{i,a,l}\) 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)];
- \(P_{imm,\text{msw}}^{i,a,l}\) 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 water)];
- \(C_{\text{dom}}^{i,l}\) is the concentration of radionuclide \(i\) in domestic water for lifestyle \(l\) [Bq/kg water];
- and
- \(C_{\text{msw}}^{i}\) is the concentration of radionuclide \(i\) in the main surface water feature [Bq/kg water].

The transfer parameter from domestic water concentration to water immersion dose rate is given as follows:

\[
P_{\text{imm,dom}}^{i,a,l} = (f_{\text{bath}} \cdot OF_{\text{bath}}^{i,a} + OF_{\text{pool}}^{i,a}) \cdot DCF_{\text{imm,wat}}^{i,a} \tag{5-64}
\]

Where,

- \(P_{\text{imm,dom}}^{i,a,l}\) 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)];
- \(f_{\text{bath}}\) is the correction factor to account for the finite size of the bath [-];
- \(OF_{\text{bath}}^{i,a}\) is the bath occupancy factor [-];
- \(OF_{\text{pool}}^{i,a}\) is the pool occupancy factor for lifestyle \(l\) [-]; and
- \(DCF_{\text{imm,wat}}^{i,a}\) is the dose conversion coefficient for water immersion for radionuclide \(i\) [(Sv/a)/(Bq/kg water)].

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

\[
P_{\text{imm,msw}}^{i,a,l} = OF_{\text{sw}}^{i,a} \cdot DCF_{\text{imm,wat}}^{i,a} \tag{5-65}
\]

Where,

- \(P_{\text{imm,msw}}^{i,a,l}\) 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 water)];
is surface water occupancy factor [-]; and

DCF_{imm,\text{wat}} is defined above.

5.12.3.3 Groundshine Dose Rates

The dose rate due to groundshine is expressed as follows:

\[ D_{\text{gshine}}^{i,a,l} = P_{\text{gshine}}^{i,a,l} \cdot \max_f \{ C_{\text{soil}}^{i,f,l} \} \]  \hspace{1cm} (5-66)

Where,

- \( D_{\text{gshine}}^{i,a,l} \) is the groundshine human dose rate for radionuclide \( i \), age group \( a \), and lifestyle \( l \) [Sv/a];
- \( P_{\text{gshine}}^{i,a,l} \) is the transfer parameter for soil concentration to groundshine dose rate for radionuclide \( i \) for age group \( a \) and lifestyle \( l \) [(Sv/a)/(Bq/kg soil-dw)]; and
- \( C_{\text{soil}}^{i,f,l} \) is the concentration of radionuclide \( i \) in the soil of field \( f \) for lifestyle \( l \) [Bq/kg soil-dw].

The transfer parameter from soil concentration to groundshine dose rate [(Sv/a)/(Bq/kg)] is defined as follows (Equation 6-80 of CSA 2014):

\[ P_{\text{gshine}}^{i,a,l} = OF_{\text{area}} \cdot f_r \cdot \left[ OF_{\text{out}}^l + (1 - OF_{\text{out}}^l) \cdot S_g \right] \cdot Z_s \cdot \rho_{\text{soil}} \cdot DCF_{g}^{i,a} \]  \hspace{1cm} (5-67)

Where,

- \( P_{\text{gshine}}^{i,a,l} \) is the transfer parameter for soil concentration to groundshine dose rate for radionuclide \( i \) for age group \( a \) and lifestyle \( l \) [(Sv/a)/(Bq/kg soil-dw)];
- \( OF_{\text{area}} \) is the area occupancy factor [-];
- \( f_r \) is the dose reduction factor to account for non-uniformity of the grounds surface [-];
- \( OF_{\text{out}}^l \) 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];
- \( DCF_{g}^{i,a} \) is the dose conversion coefficient for an infinite plane ground deposit for radionuclide \( i \) and age group \( a \) [(Sv/a)/(Bq/m²)]; and
- \( \rho_{\text{soil}} \) is the soil density [kg/dw/m³].

5.12.3.4 Beachshine Dose Rates

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

\[ D_{\text{bshine}}^{i,a,l} = P_{\text{bshine}}^{i,a,l} \cdot C_{\text{sed}}^i \]  \hspace{1cm} (5-68)

Where,
\( D_{\text{bshine}}^{i,a,l} \) is the beachshine human dose rate for radionuclide \( i \), age group \( a \), and lifestyle \( l \) [Sv/a];

\( P_{\text{bshine}}^{i,a,l} \) 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 sediment-dw)], and

\( C_{\text{sed}}^{i} \) is the concentration of radionuclide \( i \) in sediment [Bq/kg sediment-dw].

According to Equation 7-26 from Clause 7.10.1 of CSA (2014), \( P_{\text{bshine}}^{i,a,l} \) is defined as follows:

\[
P_{\text{bshine}}^{i,a,l} = O_{\text{shore}}^{l} \cdot W_{S} \cdot f_{d} \cdot \text{DCF}_{\text{sed}}^{i,a}
\]

Where,

\( P_{\text{bshine}}^{i,a,l} \) 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 sediment-dw)],

\( O_{\text{shore}}^{l} \) 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

\( \text{DCF}_{\text{sed}}^{i,a} \) is the dose conversion coefficient for uniformly contaminated sediment for radionuclide \( i \) and age group \( a \) [(Sv/a)/(Bq/kg sediment-dw)].

### 5.12.4 Total Dose Rate

The total dose rates for each lifestyle and each age group is the sum of dose contributions from all pathways described above in Sections 5.12.1 to 5.12.3 for all radionuclides, namely:

\[
D_{\text{tot}}^{a,l} = \sum_{i} D_{\text{ing}}^{i,a,l} + D_{\text{inh}}^{i,a,l} + D_{\text{imm,air}}^{i,a,l} + D_{\text{imm,wat}}^{i,a,l} + D_{\text{gshine}}^{i,a,l} + D_{\text{bshine}}^{i,a,l}
\]

### 5.13 Concentration of Non-Radiological Species

For each of the media (surface soil, surface water, well, sediment and air), the concentration of non-radiological species is determined by summing the contribution of all isotopes of each element. Thus:

\[
C_{m}^{k} = \sum_{j \in i} C_{m}^{j}
\]

Where,

\( C_{\text{media}}^{k} \) is the concentration in medium \( m \) of element \( k \) [mol/[unit volume or mass]]; and

\( C_{m}^{j} \) is the concentration in medium \( m \) of species \( j \) [mol/[unit volume or mass]].
6. SUMMARY

In summary, this report describes the theory for the Integrated System Model (ISM) v1.0 a system model designed to assess the postclosure safety of a deep geologic repository for used nuclear fuel. The system model is composed of a series of linked models representing the near field (ISM-NF), the geosphere (ISM-GEO) and the biosphere (ISM-BIO). Key features and processes in the ISM-NF model include:

- 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.

Key features and processes in the ISM-GEO model include:

- 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.

Key features and processes in the ISM-BIO model include:

- 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).
In general, the ISM v1.0 theory is largely consistent with the approach and theory from the SYVAC3-CC4 (previous generation) system model (NWMO, 2012). However, the ISM v1.0 model has several notable improvements including:

- Higher fidelity between 3D representation of the nearfield and repository design;
- More robust representation of used fuel container failure and subsequent release of species from a failed container;
- Higher fidelity between 3D representation of the geosphere and repository sites;
- Calculation of the groundwater flow field in the geosphere;
- Greater consistency with CSA (2014) biosphere model;
- Additional critical group lifestyle (hunter-gatherer); and
- Additional critical group dose receptors (child, infant).
REFERENCES


COMSOL. 2018. COMSOL v5.4 Subsurface Flow Module User's Guide. Massachusetts, USA.


Quintessa. 2018. AMBER 6.3 User Guide. Henley-on-Thames, United Kingdom.

