



ARBEITSBERICHT NAB 23-25

Biosphere modelling for C-14:
Description of the Nagra model

October 2023

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

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Biosphere modelling for C-14:
Description of the Nagra model

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This report was prepared on behalf of Nagra. The viewpoints presented and conclusions reached are those of the author(s) and do not necessarily represent those of Nagra.

Summary

Nagra uses a compartment model for representing the distribution of radionuclides in the biosphere following release from a deep geological repository and for calculating potential effective radiation doses to persons. The compartment model is implemented as the Swiss Biosphere Assessment Code (SwiBAC) and adopts equilibrium assumptions for radionuclide distribution between solid phases, liquid phases and uptake by crops. Such assumptions are suitable for biosphere modelling of most radionuclides relevant to geological disposal.

For C-14, a more specific modelling approach is appropriate. This report documents the model that is used by Nagra to represent the distribution of C-14 in the biosphere. The conceptual and mathematical model for evaluating the transfer and accumulation of C-14 released to a local aquifer-soil-crop-atmosphere system is presented. The data for the model are described and justified, along with details of numerical implementation and illustrative calculations. The model draws on discussions and comparisons relating to C-14 modelling made within the international BIOPROTA forum and modelling and associated research undertaken by other radioactive waste management organisations.

The model assumes that C-14 is distributed in the same way as stable carbon and is hence based on masses and fluxes of stable carbon between various carbon pools. The mass balance demonstrates the dominance of exchanges between soil solution, soil gas and the exchanges of stable carbon between the soil, plant canopy and above-canopy atmosphere. Organic matter represents the major carbon pool within the topsoil in comparison with the amount in exchangeable inorganic form.

Illustrative calculations demonstrate a timescale of several hundred years to equilibrium, reflecting the assumed turnover rate of carbon within the local aquifer. The degree of atmospheric mixing within the plant canopy atmosphere means that the small amount of plant carbon derived from root uptake of dissolved inorganic carbon dominates as a pathway for C-14 uptake by plants for a source term to the soil.

Nagra's biosphere model for C-14 model is used to calculate the following effective parameter values needed to represent the behaviour of C-14 within SwiBAC:

- effective solid/liquid distribution coefficients for the soil compartments, the variably saturated zone and the local aquifer;
- the loss term from the topsoil to reflect degassing losses to the atmosphere and losses through harvested crops; and
- effective soil-to-plant concentration ratios for the different crops considered.

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1 Introduction

Nagra is responsible for the management and disposal of radioactive waste arising in Switzerland in a way that ensures the long-term protection of humans and the environment. The Swiss radioactive waste management programme foresees deep geological disposal in two types of facility, one facility for high-level radioactive waste (HLW repository) and one for low- and intermediate-level radioactive waste (L/ILW repository), co-located at a single site (Nagra 2021). There is potential for some small fraction of the radioactivity originating or in-grown from the disposed waste to reach the surface and near-surface environment (referred to as the biosphere) on extremely long timescales. Nagra needs to assess potential radiological exposures in the biosphere for comparison against regulatory criteria.

C-14 may be released from a deep geological disposal facility either dissolved in groundwater, or in the gas phase, with advection of accompanying bulk gases. Once in the deep groundwater system, C-14 in the gas phase is taken to dissolve in solution (Nagra 2024a). The principal source to the biosphere is, therefore, C-14 dissolved in groundwater reaching shallow local aquifers, consistent with other radionuclides.

Nagra uses a compartment model for representing the behaviour of radionuclides released from a deep geological repository to the biosphere. The model is implemented as the SwiBAC code (Nagra 2024b) and adopts equilibrium assumptions for radionuclide distribution between solid and liquid phases and uptake by plants. Such assumptions are appropriate for biosphere modelling of most radionuclides relevant to geological disposal, given the long time periods being considered. However, C-14 represents a radioisotope of an element that is a fundamental building block of biological systems and for which such assumptions are more difficult to justify (Sheppard & Thorne 2005).

Intercomparison of models for C-14 in the biosphere has formed part of the focus of successive projects and workshops within an international collaborative project, BIOPROTA (Limer 2019). Such comparisons demonstrate the importance of representing the exchange of carbon between the soil, the plant canopy atmosphere and the atmosphere above the canopy. This has highlighted potentially significant conservatism in the representation of the plant canopy atmosphere and has led to biosphere models for C-14 that have refined the representation of these features and processes (e.g. Thorne & Walke 2013, Saetre et al. 2013, and Hoch 2014).

This report documents the conceptual and mathematical model along with data used by Nagra to represent the behaviour of C-14 in the biosphere. It also comprises details of numerical implementation, illustrative calculations and some conclusions.

The report builds on and updates the previous assessment approach used by Nagra for representing C-14 in the biosphere (Walke et al. 2013). In particular, the pessimistic way in which the plant canopy atmosphere had previously been represented has been updated, consistent with the most recent international research and the updated representation of C-14 in other assessment programmes.

The report is structured as follows:

- the conceptual model is described in Section 2;
- the mathematical model is described in Section 3;
- the parameter values and associated discussion are presented in Section 4;
- implementation is discussed in Section 5;
- illustrative calculations are presented in Section 6, including comparison against Nagra's previous model for C-14 in the biosphere;

- the exchange of information between the C-14 model and Nagra's biosphere modelling code SwiBAC is discussed in Section 7, including comparison of the effect of the updated model on the biosphere dose conversion factor for C-14;
- conclusions are then drawn in Section 8.

2 Conceptual model

Fundamental assumptions are that:

- the timescale of the release of C-14 to the biosphere is sufficiently long that its distribution reaches steady state;
- photosynthetic isotopic fractionation between C-14 and stable carbon (C-12) is relatively unimportant, the maximum discrimination being about 5%¹ (NCRP 1984);
- the biosphere system is in steady state, such that stable carbon does not accumulate or deplete in the parts of the biosphere of relevance.

2.1 Basis

Radiocarbon from the repository is principally taken to reach the biosphere as carbon dissolved in water in the form of radiolabelled:

- carbon dioxide or bicarbonate;
- methane; or
- organic molecules (i.e. carboxylic acids).

It is noted that some fraction of dissolved ¹⁴C-methane or ¹⁴C-carbon dioxide may form a gas phase again in the shallow aquifer and/or in the deeper aquifer pathway, depending on its concentration and the local pressure, temperature and salinity conditions. The extent to which C-14 may form a gas phase after migrating away from the repository in aquifer pathways is uncertain and the modelling described below is based on its remaining in solution. However, bounding consideration is given to release to gas phase in Section 7.2.

Processes important to the assessment of potential dose consequences associated with release of C-14 to the biosphere in the long-term centre around the oxidation of methane in the soil, release of carbon dioxide to the plant canopy atmosphere, exchanges between the plant canopy atmosphere and the wider atmosphere, and the degree of plant uptake of carbon from the canopy atmosphere. These processes, therefore, are the focus for the following discussion, which provides the scientific basis for the subsequent conceptual model (Section 2.2).

Methane can be oxidised to carbon dioxide both in oxygenated regions of the aquifer and in unsaturated soils and C-14 originally incorporated in the methane will become incorporated in carbon dioxide². Observed oxidation rates for methane in agricultural and pasture soils are in the order of 0.014 to 0.84 mg m⁻² d⁻¹ (Thorne & MacKenzie 2005). In a more recent review, Shaw & Thorne (2016) reported that methane oxidation proceeds at ambient atmospheric concentrations in a wide range of agricultural, grassland and forest soils. Over all the land use types considered, the geometric mean oxidation rate was 0.57 mg m⁻² d⁻¹ and the highest median rate recorded in a single study was about 3.6 mg m⁻² d⁻¹. Oxidation rates are rather lower in agricultural soils than in grassland or forest soils and a value of about 0.2 mg m⁻² d⁻¹ is more typical of such soils. This latter value is statistically indistinguishable from the geometric mean oxidation rate that was measured in field experiments conducted at the University of Nottingham (Shaw & Thorne 2016). The typical threshold concentration below which methane oxidation ceases has been determined

¹ The isotopic fractionation varies between plant species and differs greatly between C₃ (most food crops) and C₄ (sugar cane, maize) pathways for photosynthesis. The maximum discrimination occurs in the C₃ plant pathway (NCRP 1984).

² With respect to direct uptake of C-14 with methane in drinking water, the exposure model does not distinguish between the chemical form of C-14, effectively assuming that all are 100% absorbed.

experimentally to be substantially below the ambient (free atmosphere) concentration of 1.8 ppmv, although higher thresholds have been recorded in some studies (Shaw & Thorne 2016). Organic molecules dissolved in water will also be oxidised to CO₂ by micro-organisms in the biosphere, for example, the behaviour of ethylene and acetylene in the soil zone is discussed in Thorne (2005a). In the context of plant uptake of C-14, it is conservatively assumed that all of the C-14 entering the soil is available as carbon dioxide or bicarbonate, so other forms are not discussed further.

Terrestrial plants derive most of their carbon from the atmosphere. Aquatic plants may derive a significant part from the water depending on the fraction of the plant that is submerged. However, local aquatic products are traditionally only of minor importance in the Swiss diet, so they are not included in the model.

Soil organic matter is mainly derived from plant material (plant parts within the soil – termed roots here – and above-ground plant material) or animal excreta, which is also indirectly plant-derived material. The different forms of organic matter can be transformed or decomposed at different rates, as discussed in the context of detailed models for carbon in the soil, such as the RothC model³ (Coleman & Jenkinson 1999, Jenkinson & Coleman 2008).

Solid inorganic carbon in soils is mainly present as carbonates in amorphous and crystalline forms. The rate of exchange between dissolved carbon dioxide / bicarbonate and solid inorganic carbon can vary between soils, within a soil with time and also between different forms of solid carbonate (the exchange rate being highest for amorphous carbonate). The steady-state condition of this exchange can be described by a solid / liquid distribution coefficient.

Another important carbon component in soil is carbon in plant roots. Carbon can be released from roots in the form of an exudate of organic compounds (e.g. as a complexing agent for iron), as CO₂ and bicarbonate from respiration, or by decomposition of dying roots and of sloughed-off root material. Bicarbonate can be both released from and absorbed by roots to keep electro-neutrality when different equivalents of nutrient cations and anions are absorbed by roots. Literature data indicate that a small fraction of the carbon in roots or in the total plant could be derived from the soil, whereas most is derived from photosynthesis by the leaves. Inorganic carbon may also be transported with the water flux in the xylem upwards and assimilated in aerial plant parts (Evenden et al. 1998, Milton et al. 1998).

The carbon from the degradation of organic matter in soil (mineralisation processes) can either be transported downwards with soil water (percolation) or released into the soil gas phase as CO₂. From the soil gas phase, the CO₂ can be released into the air layer above the soil due to diffusion or because of pressure variations in the atmosphere that pump air into or out of the soil.

The major input of carbon into the soil-plant system is through assimilation of atmospheric CO₂ in the plant canopy by the plant. This canopy-atmosphere carbon is partly derived from CO₂ released from the soil but is also partly brought into the canopy by wind and other atmospheric exchange processes. The ratio between atmospheric and soil-derived carbon depends on atmospheric mixing processes and critically on the density of the plant canopy and its structure, which in turn depend on the mix of plants present and their morphology. The time-dependent development of the canopy is also an important consideration. Hence, there is an important linkage between the canopy structure and carbon dioxide transport and uptake by photosynthesis. The denser the canopy, the greater the degree of hold up of carbon dioxide released from the

³ The model RothC-26.3, (Coleman & Jenkinson 1999, Jenkinson & Coleman 2008) considers resistant plant material, decomposable plant material, microbial mass, humified organic matter and inert organic matter as forms of organic carbon in non-water-logged soils.

ground, but also the greater the degree of light attenuation in the upper part of the canopy, which reduces photosynthetic rates at the lower levels where soil-derived carbon dioxide concentrations are highest.

In the plant canopy, transport of gaseous carbon dioxide results from a combination of the processes of advection, turbulent mixing and diffusion. The relative importance of these processes varies within the plant canopy both in respect of height above the ground surface and in relation to meteorological conditions. Close to the ground surface, the air will be slow moving and diffusion may make a substantial contribution to the transport of gaseous carbon dioxide. However, higher in the canopy, the effects of wind movement above the canopy will be reflected in disturbance of the air within the canopy and lead to turbulent mixing. This can be treated as a dispersive process and modelled in the same way as diffusion. Indeed, diffusion and dispersion can be treated as a single, combined process, modelling using a Fickian approach to dispersion.

The reason for modelling the transport of C-14 bearing carbon dioxide through the plant canopy is to estimate the average specific activity of the carbon dioxide taken up by plants and used in photosynthesis to produce biomass. This average depends on the vertical profile of carbon dioxide specific activity and on variations in the rate of photosynthesis with height. In turn, the latter depends on light intensity, which varies with depth of penetration into the canopy because of shading. In practice, this level of detailed information is unlikely to be available and it is reasonable to approximate the system in terms of vertically integrated “pools” of carbon and C-14, and a vertically integrated rate of production of plant biomass.

A fraction of the carbon assimilated by the plant through photosynthesis will be lost by respiration, either as maintenance respiration or for energy required for the transformation of plant compounds (e.g. carbohydrates into lipids). Respiration occurs both in the above-ground plant and the roots. Photosynthesis occurs only when plants are illuminated, whereas respiration occurs both during the day and at night. Therefore, the net carbon balance of plants varies diurnally, with uptake dominating during the day and loss at night.

Above-ground plant material or roots (and tubers) can be harvested for consumption by humans or animals. For annual arable crops, the roots will, when not harvested, be left in the soil and also the non-harvested part of the above-ground plant may be left on or ploughed into the soil. Different considerations apply to perennial crops (e.g. tree fruits), where much of the C-14 inventory may be retained in woody parts for many years. For pasture, grazing might be considered as quasi-continuous cropping.

2.2 Model outline

C-14 is taken to behave in the soil-plant system in the same manner as stable carbon without isotopic fractionation. Therefore, the model is defined in terms of carbon pools and carbon transfers that are considered explicitly.

The conceptual model for carbon is illustrated in Fig. 2-1, with each box representing a pool of carbon that is explicitly considered. There is consistency in the structure of the aqueous phase pools highlighted in light blue in Fig. 2-1 and the structure of the SwiBAC model (Nagra 2024b), enabling dimensions and water flows to be shared between the models. Transfers of solid material considered in SwiBAC are neglected because the migration of C-14 between the soil, aquifer and surface water is taken to be dominated by that in the aqueous and gaseous phases rather than the relatively small component that might become associated with solid inorganic material.

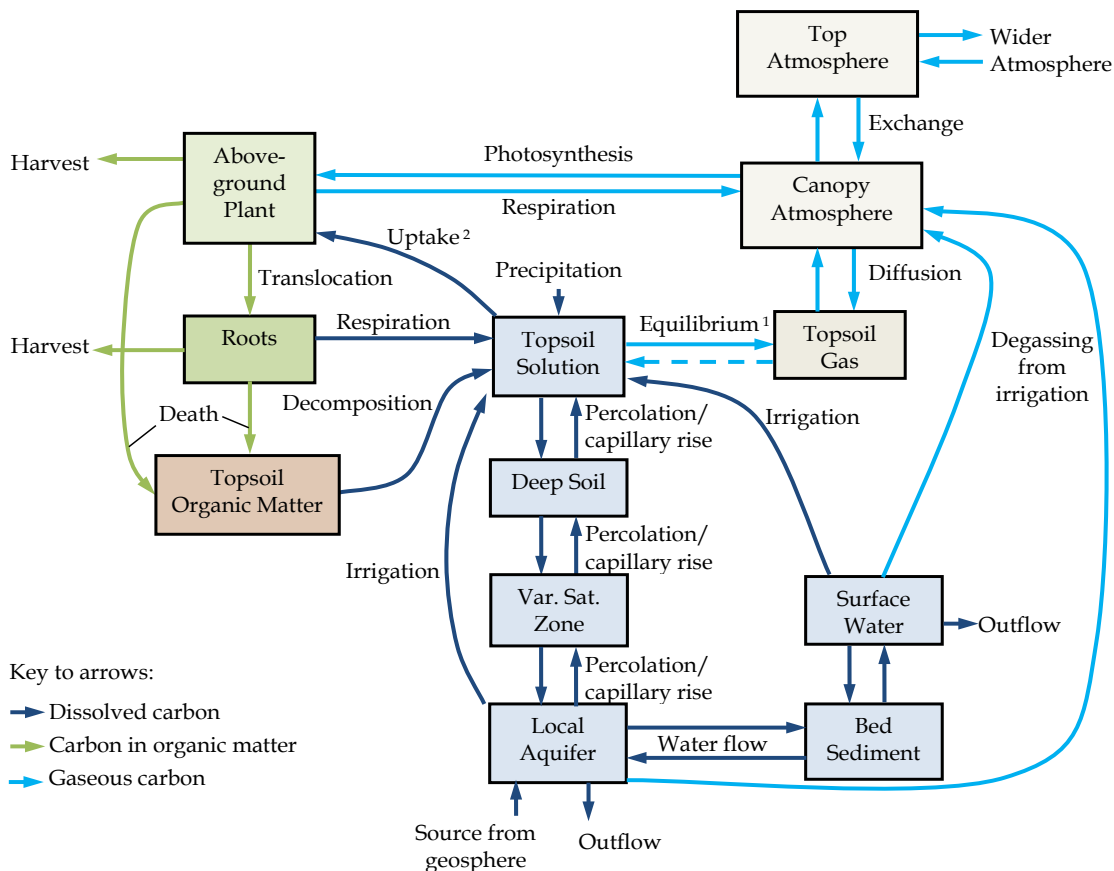


Fig. 2-1: Conceptual model of carbon dynamics

Numbered footnotes: (1) Whilst conceptually carbon can be exchanged between the soil gas and soil solution, in practice release from the soil solution to soil gas is taken to dominate. (2) Carbon taken up from the topsoil solution by the plant for use in photosynthesis within the plant leaves is assumed not to interact with the roots.

The underlying water flows are illustrated for the reference biosphere case in Nagra (2024b). Names of carbon pools are capitalised because they support indices in the mathematical model.

The source term considered is deep groundwater containing C-14 which discharges into a shallow local aquifer and/or C-14 reaching the local aquifer in the gas phase and being dissolved in the shallow groundwater. The potential consequence of degassing of ¹⁴C-methane and ¹⁴C-carbon dioxide from groundwater can be bounded by direct release to the topsoil solution and topsoil gas and is explored further in Section 7.

Endpoints of the model calculations are C-14 concentrations and the C-14 specific activities (i.e. Bq kg⁻¹) in the different compartments.

Dissolved inorganic carbon in topsoil solution, deep soil solution, variably saturated zone and the local aquifer is explicitly considered. Soil organic matter is explicitly considered in the topsoil⁴.

⁴ Whilst it is possible to distinguish different forms of organic carbon within the soil (e.g. Coleman & Jenkinson 1999), a single compartment for all kinds of organic carbon is considered appropriate for post-closure safety assessments, given that the key processes lie elsewhere within the model, in particular in exchanges between the soil gas, the canopy atmosphere and above canopy atmosphere. Although some organic matter occurs in soil at depth, most of it is concentrated in the topsoil.

Carbon in plant roots within the topsoil is explicitly represented, as is carbon in the above-ground plants. Carbon in soil gas is explicitly represented⁵.

The atmosphere is represented with:

- a compartment for the air within the plant canopy;
- a compartment representing the atmosphere immediately above the plant canopy, which is referred to as the top atmosphere; and
- the atmosphere outside the top atmosphere compartment, which is represented as a sink for C-14 and is referred to as the wider atmosphere.

Dissolved inorganic carbon is explicitly represented within surface water and river-bed sediment. These compartments are included within the SwiBAC model, with associated water and solid material transfers, and are thus needed in the model for C-14 to facilitate its integration with SwiBAC. However, the principal focus of the model for C-14 is its behaviour in the soil-plant system, so the surface water and riverbed sediment compartments are represented as relatively inert parts of the system with respect to carbon relevant processes, although there is potential for a loss of C-14 from surface water to the atmosphere due to degassing. However, such degassing is primarily relevant to lakes and mires with long water turnover times. In rapidly flowing rivers and lakes with short water residence times, carbon losses are governed by water turnover rather than degassing. In view of this, it is slightly cautious to neglect degassing when modelling carbon transport in surface waters.

Inorganic carbon is transported with the water fluxes between the compartments. The carbon dissolved in precipitation and irrigation water is assumed to be transferred directly to the topsoil solution with no interaction with the plant canopy⁶. There is potential for inorganic carbon in irrigation water to be released to the atmosphere due to degassing.

Although it is considered a relatively minor route for provision of carbon for photosynthesis, uptake of dissolved inorganic carbon by the plant roots is modelled by a flux directly from topsoil solution to the above-ground plant, assuming that this inorganic carbon is transported with the water flux through the xylem without interaction with the roots to the above-ground plant and is assimilated in the leaves into organic carbon by photosynthesis. Root respiration and decomposition of soil organic matter are assumed to add inorganic carbon to the topsoil solution. The effect of dissolved inorganic carbon produced by the respiration of roots and the decay of organic matter on chemical processes involving CaCO_3 is not taken into account. Consistent with the assumption of a steady state, the soil chemistry is assumed not to change.

Soil gas is assumed to be in equilibrium with soil solution. Whilst, conceptually, carbon can be exchanged between the soil gas and solution, in practice, release from the soil solution to soil gas is taken to dominate.

Transport from the soil gas to the canopy atmosphere is treated as a diffusive process. In principle, it will comprise both molecular diffusion and the effects of atmospheric pumping due to variations in atmospheric pressure. Considering molecular diffusion alone, the characteristic timescale for transport through the unsaturated soil, T (s), is given by Hoch [2014] (derived from Equation 4.10):

⁵ In the biosphere assessment model implemented by SwiBAC, the topsoil is represented by a single compartment while there are three (Topsoil Organic Matter, Topsoil Solution and Topsoil Gas) in the discussed C-14 model.

⁶ Although foliar uptake is conceivable, outgassing will tend to rapidly release most of the C-14 and little will pass through the stomata.

$$T = \frac{L^2 \theta_w}{D} \quad [-] \quad (1)$$

L $[m]$ is the depth of the unsaturated layer,
 θ_w $[-]$ is the water-filled porosity of the soil,
 D $[m^2 s^{-1}]$ is the molecular diffusion coefficient.

For illustrative purposes, based on Hoch (2014), taking $\theta_w = 0.5$ for a well-drained agricultural soil, $L = 0.5$ m and $D = 1.6 \cdot 10^{-5} \text{ m}^2 \text{ s}^{-1}$, $T = 0.125/1.6 \cdot 10^{-5} = 7.8 \cdot 10^3 \text{ s}$ (2.2 h).

This timescale suggests that the inclusion of dispersion due to pressure changes would not markedly affect the effective diffusion coefficient. However, the model is defined in a general form such that the diffusion coefficient D can be used to represent the overall effect of molecular diffusion plus turbulent dispersion in the soil layer. Alternatively, D can be decreased to represent the effects of tortuosity in the soil pores, which has an inhibitory effect on both molecular diffusion and turbulent dispersion.

Advective and turbulent mixing occurs between the canopy atmosphere and the top atmosphere compartment⁷. Diffusive/dispersive exchange is taken to operate as a loss term for radiocarbon from the top atmosphere to the wider atmosphere above, and horizontal advective transport is taken to operate from the top atmosphere to the wider atmosphere, which also removes radiocarbon from the model.

Inorganic carbon is absorbed by the above-ground plant from the air within the canopy and assimilated into organic plant material by photosynthesis. A reverse flux from the above-ground plant to the air within the canopy is caused by respiration. The long-term nature of C-14 releases to the biosphere from a geological disposal facility means that the diurnal cycle of photosynthesis and respiration does not need to be explicitly represented; rather, average rates are sufficient.

Instead of a photosynthesis model to predict the production of plant material, the annually produced plant material (a measured parameter) is used. This helps ensure consistency with parameter assumptions in Nagra's general biosphere modelling (Nagra 2024b). The fraction lost by respiration is added to this net plant production to obtain the gross plant assimilation rate.

A part of the organic carbon assimilated in the above-ground plant is transferred to the roots. Organic carbon is removed from the system by harvest of above-ground plants and roots. The organic carbon in the above-ground plant and roots remaining after harvest minus respiration is added to the topsoil organic matter. To keep a constant concentration of soil organic matter, the annual production of plant derived organic matter is decomposed at the same rate as it is added.

⁷ This is a key improvement in comparison to Walke et al. (2013). In the previous model, the plant canopy was taken to be diffusively dominated up to the zero-displacement plane. That assumption was acknowledged as being pessimistic at the time and is replaced here with the assumption that turbulent mixing extends further through the plant canopy atmosphere, on the basis discussed in Section 2.2.

3 Mathematical model

The mathematical model for C-14 in the biosphere is based on the structure of carbon pools discussed in the previous section – each represented by a compartment. A compartment can be described here as a local entity, whose properties are determined by a set of local parameters, and which is associated with a static inventory of stable carbon and a time-variant one of C-14.

The model for stable carbon consists of

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

The stable carbon fluxes into and out of each compartment must balance to maintain the time invariant stable carbon amounts.

The stable carbon amounts and fluxes provide transfer rates for stable carbon around the biosphere system. The same transfer rates apply for C-14, such that the behaviour of C-14 within the biosphere system can be modelled dynamically.

The mathematical model can be distinguished into that associated with calculating stable carbon inventories in each compartment (Section 3.2), that associated with calculating fluxes of stable carbon between the compartments (Section 3.3) and that for interpreting the resulting transfer rates for C-14 (Section 3.4)⁸. The model can be used to determine effective soil-to-plant concentration ratios, soil solid / liquid partitioning coefficients and volatilisation rates for C-14, which can be used in the SwiBAC biosphere model (Section 3.5).

The spatial extent of the model is the same as that for Nagra's general biosphere modelling, which is the area of the local aquifer in a valley bottom that receives the potentially contaminated groundwater (Nagra 2024b).

The nomenclature adopted for the compartments considered is given in Tab. 3-1. The compartment Elsewhere serves as a generic sink, which gathers losses of carbon in the system by harvest of crops and outflow of groundwater.

⁸ Note that further discussion relating to specific parameters is included in the definition of parameter values in Section 4.

Tab. 3-1: Compartments of the C-14 model

Compartments with a two letter index are part of the C-14 model while the Topsoil, T, is to be seen as the corresponding compartment of the SwiBAC model or as an ensemble of the three compartments TS, TO and TG. The Wider Atmosphere, AW, is part of the conceptual model but is not implemented in the code as a compartment of its own; instead it is attributed to the generic sink compartment Elsewhere.

Compartment	Index	Compartment	Index
Local Aquifer	LA	Roots	PR
Surface Water	WS	Above-ground Plant	PA
Bed Sediment	WB	Canopy Atmosphere	AP
Variably Saturated Zone	VZ	Top Atmosphere	AT
Deep Soil	DS	Wider Atmosphere	AW
Topsoil	T	Contaminated Source	SC
Topsoil Solution	TS	Uncontaminated Source	SU
Topsoil Organic Matter	TO	Elsewhere	EW
Topsoil Gas	TG		

3.1 Compartment modelling approach

The inventories and the fluxes of stable carbon within and between the compartments are assumed to be time-independent. C-14 is introduced via an inflow of contaminated groundwater to the local aquifer. The mathematical representation of the inter-compartmental transfer processes takes the form of a matrix of transfer coefficients. This allows the changes in compartment amounts to be represented using a set of first-order linear differential equations. For the i^{th} compartment, the rate at which the compartment inventory of contaminants (including C-14) changes with time is given by:

$$\frac{dN_i}{dt} = \left(\sum_{j \neq i} \lambda_{ji} N_j + \sigma_{MN} \lambda_N M_i + S_{N,i} \right) - \left(\sum_{j \neq i} \lambda_{ij} N_i + \lambda_N N_i \right) \quad [Bq \ a^{-1}] \quad (2)$$

where:

i and j

indices denoting the corresponding compartments,

N and M $[Bq]$

amounts of contaminants N and M in a compartment (M is the precursor of N in a decay /degradation chain),

$S_{N,i}$ $[Bq \ a^{-1}]$

time-dependent external source of contaminant N , i. e. C-14, to compartment i ,

λ_M and λ_N $[a^{-1}]$

decay constant for contaminants M and N respectively,

σ_{MN} $[-]$

branching ratio for decay from contaminant M to N ,

λ_{ji} and λ_{ij} $[a^{-1}]$ transfer coefficient representing the gain and loss of contaminant N from compartment i by transfer from and to compartment j , respectively⁹.

The derivation of the transfer rates for C-14 from the stable carbon model is described in the following sections. For C-14, in-growth from a parent radionuclide, which is included in Equation 1, is not relevant. The solution of the linear system of ordinary differential equations given above provides the time-dependent inventory of C-14 in each compartment. From the compartment sizes, estimates of the associated concentrations can then be made.

The implementation of the model is based on the generic compartment modelling code AMBER (Quintessa 2022).

3.2 Stable carbon masses

The amount of exchangeable stable inorganic carbon in the Local Aquifer, Variably Saturated Zone, Deep Soil and Topsoil Solution is given by Equation 3. Note that for the Topsoil Solution, the contributing parameters relate to the Topsoil as a whole:

$$AC_i = f_{EC} f_{CC,i} C f_{CC} V_i \rho_{b,i} \quad [kg_C] \quad (3)$$

i compartment index LA, VZ, DS or TS ,
 f_{EC} $[-]$ exchangeable carbonate as a mass fraction of the total carbonate, f_{CC} $[kg_{CaCO_3} kg^{-1}]$ mass fraction of the compartment solid as calcium carbonate,
 $C f_{CC}$ $[kg_C / kg_{CaCO_3}]$ mass fraction of carbon in calcium carbonate,
 V $[m^3]$ volume of the compartment,
 ρ_b $[kg m^{-3}]$ dry bulk density of the compartment given by:

$$\rho_{bi} = (1 - \theta_{ti}) \rho_{gi} \quad [kg m^{-3}] \quad (4)$$

θ_t $[-]$ total porosity of the compartment,
 ρ_g $[kg m^{-3}]$ grain density of solid material in the compartment.

The amount of stable carbon in Topsoil Organic Matter is given by:

$$AC_{TO} = f_{OM,T} C f_{OM} V_T \rho_{b,T} \quad [kg_C] \quad (5)$$

$f_{OM,T}$ $[kg kg^{-1}]$ organic matter content of the topsoil solid as a mass fraction,
 $C f_{OM}$ $[kg_C kg^{-1}]$ mass fraction of carbon in organic matter,
 V_T $[m^3]$ volume of Topsoil.

⁹ Transfers out of the system can be represented by transferring contaminants to a “sink” compartment that is not used in calculating endpoints, i.e. transient inventories of C-14.

The amount of stable carbon in Surface Water and Bed Sediment is given by¹⁰:

$$AC_i = Cf_{w,i} \theta_{w,i} V_i \quad [kg_C] \quad (6)$$

i compartment index *WS* or *WB*,

θ_w [-] volumetric moisture content,

Cf_w [$kg_C m^{-3}$] carbon content in the water.

The amount of stable carbon in Roots and Above-Ground Plant for a given crop type is:

$$AC_i = A_f B_i Cf_{OM} \quad [kg_C] \quad (7)$$

i compartment index *PR* or *PA*,

A_f [m^2] area of the agricultural land,

B [$kg m^{-2}$] standing biomass of root or above-ground organic matter per unit surface area.

Note that the standing biomass is taken to have the same value as the annual net dry weight yield of plant organic matter. This assumption does not allow for multiple harvests per year, which is considered appropriate for Central Europe.

Note also that the carbon fraction in soil organic matter is taken to be the same as that in standing biomass, expressed on a dry mass basis. This is considered reasonable, as the model assumes that soil organic matter degrades uniformly. However, in practice, there may be some change in the carbon to dry mass ratio during mineralisation of soil organic matter.

It is assumed that the concentrations of stable carbon in the plant canopy atmosphere are the same as in the general atmosphere; i.e. the rates of uptake and diffusive loss from soil are negligible compared with the total flux of carbon through these compartments, implying that most of the carbon within them originates from the overlying atmosphere. Therefore, the amount of stable carbon in both the Top Atmosphere and Canopy Atmosphere are given by¹¹:

$$AC_i = A_f h_i f_{CO_2} Cf_{CO_2} \quad [kg_C] \quad (8)$$

i compartment index *AT* or *AP*,

h [m] vertical thickness of the layer,

f_{CO_2} [-] volumetric fraction of CO_2 in the air above the canopy,

Cf_{CO_2} [$kg_C m_{CO_2}^{-3}$] is the mass of inorganic carbon in $1 m^3$ of CO_2 .

The vertical thickness of the Canopy Atmosphere, h_{AL} , is taken to be the same as the canopy height:

¹⁰ The principal focus of the model is on the soil-plant system, so the surface water and bed sediment are represented as relatively inert parts of the system, as described in Section 2.2.

¹¹ The plant volume is considered negligible.

$$h_{AP} = z_C \quad [m] \quad (9)$$

z_C [m] canopy height.

The top of the Top Atmosphere is taken to be at a fixed height of 10 m, z_{10} , above the ground surface. The vertical thickness of the Top Atmosphere, h_{AT} , is therefore given by:

$$h_{AT} = z_{10} - z_C \quad [m] \quad (10)$$

The concentration of stable carbon in Topsoil Gas is assumed to be higher than, but in equilibrium with, the Canopy Atmosphere, therefore the amount of carbon in the Topsoil Gas is given by:

$$AC_{TG} = E_f f_{CO_2} C f_{CO_2} (\theta_{t,T} - \theta_{w,T}) V_T \quad [kgC] \quad (11)$$

E_f [-] enhancement factor for the concentration of carbon in soil gas in comparison to the canopy atmosphere,

$\theta_{t,T}$ [-] total porosity of the Topsoil,

$\theta_{w,T}$ [-] water filled porosity (volumetric moisture content) of the Topsoil.

3.3 Stable carbon fluxes

Most of the stable carbon fluxes are explicitly parameterised and calculated. Given that the model is based on a steady-state carbon balance, the total stable carbon input and output from each compartment must balance. Therefore, some stable carbon fluxes can be calculated based on the carbon balance. The transfers that are explicitly calculated and those that are determined by the carbon balance are highlighted in Fig. 3-1.

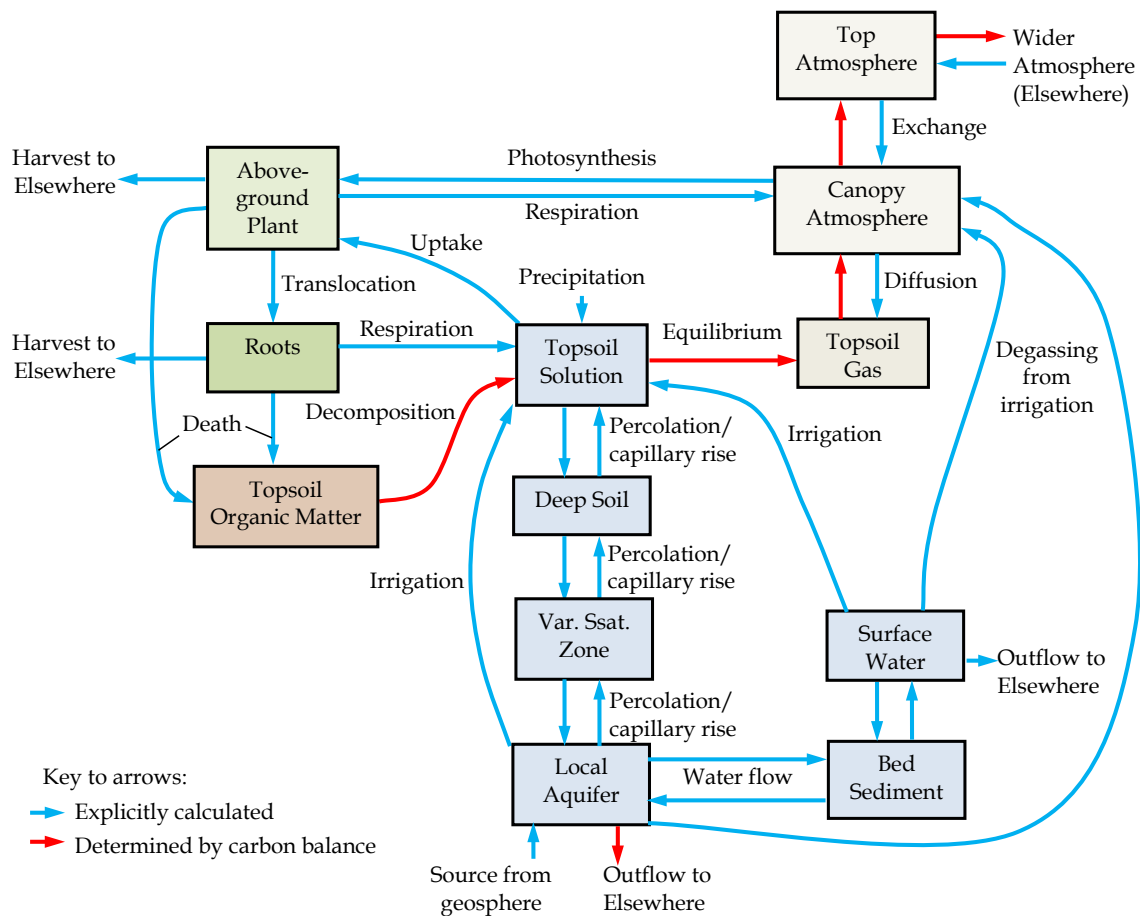


Fig. 3-1: Transfers of stable carbon / C-14 between model compartments

Transfers are explicitly calculated (blue) or determined by the carbon balance (red). The underlying water flows are illustrated for the reference biosphere case in Nagra (2024b).

Stable carbon fluxes, FC , can occur with water flow from the uncontaminated and contaminated source¹² to Local Aquifer and Surface Water, from Local Aquifer to Variably Saturated Zone, Variably Saturated Zone to Local Aquifer, Variably Saturated Zone to Deep Soil, from Deep Soil to Variably Saturated Zone, from Deep Soil to Topsoil Solution, from Topsoil Solution to Deep

¹² These represent inputs to the modelled biosphere from outside; consistent with Nagra's general biosphere modelling, these can occur to the Local Aquifer and Surface Water, compartments, see Nagra (2024b).

Soil, from Surface Water to Bed Sediment, from Bed Sediment to Surface Water, from Bed Sediment to Local Aquifer from Local Aquifer to Bed Sediment, from Local Aquifer to Elsewhere and from Surface Water to Elsewhere:

$$FC_{i,j} = F_{ij} Cf_{W,i} \quad [kg_C a^{-1}] \quad (12)$$

F_{ij} $[m^3 a^{-1}]$ water flux from compartments i to j ,
 Cf_W $[kg_C m^{-3}]$ carbon content in the water of compartment i ; note that the carbon content in Local Aquifer water is also used for transfers from uncontaminated and contaminated sources to the Local Aquifer.

The stable carbon fluxes due to irrigation from Local Aquifer to Topsoil Solution, $FC_{LA,TS}$, and from Surface Water to Topsoil Solution, $FC_{WS,TS}$, are given by:

$$FC_{LA,TS} = F_{LA,TS} Cf_{W,LA} (1 - f_{degass}) \quad [kg_C a^{-1}] \quad (13)$$

$$FC_{WS,TS} = F_{WS,TS} Cf_{W,WS} (1 - f_{degass}) \quad [kg_C a^{-1}] \quad (14)$$

$F_{LA,TS}$ $[m^3 a^{-1}]$ irrigation water flux from the aquifer to the topsoil,
 $F_{WS,TS}$ $[m^3 a^{-1}]$ irrigation water flux from the surface water to the topsoil,
 f_{degass} $[-]$ fraction of carbon content in irrigation water lost to the atmosphere due to degassing.

Any degassing from irrigation water is taken to contribute to the Canopy Atmosphere. The stable carbon fluxes from Local Aquifer to the Canopy Atmosphere, $FC_{LA,AP}$, and Surface Water to Diffusive Atmosphere, $FC_{WS,AP}$, are given by:

$$FC_{LA,AP} = F_{LA,TS} Cf_{W,LA} f_{degass} \quad [kg_C a^{-1}] \quad (15)$$

$$FC_{WS,AP} = F_{WS,TS} Cf_{W,WS} f_{degass} \quad [kg_C a^{-1}] \quad (16)$$

The stable carbon flux from the Wider Atmosphere to the Topsoil Solution, $FC_{AW,TS}$, is given by:

$$FC_{AW,TS} = d_{precipit} A_f Cf_P \quad [kg_C a^{-1}] \quad (17)$$

$d_{precipit}$ $[m a^{-1}]$ precipitation rate,
 Cf_P $[kg_C m^{-3}]$ carbon content in precipitation.

Transport vertically from the soil gas through the canopy to the atmosphere is treated using a resistance-analogue approach (consistent with Thorne & Walke 2013, and Hoch 2014).

The transport resistance across the full height of the canopy, Ω^{Canopy} , is given by¹³:

$$\Omega^{Canopy} = \frac{\ln\left(\frac{z_{Ref} - z_d}{z_{0m}}\right) \ln\left(\frac{z_{Ref} - z_d}{z_{0c}}\right)}{k^2 u_a} \quad [s \ m^{-1}] \quad (18)$$

k	$[-]$	von Kármán's constant,
u_a	$[m \ s^{-1}]$	is the wind speed at a reference height, z_{Ref} , above the ground,
z_{Ref}	$[m]$	is the reference height above the ground; this can be any specified height above the top of the canopy and does not need to be the standard 10 m height at which meteorological conditions are typically measured – here, it is taken to be the mid-point of the Top Atmosphere,
z_d	$[m]$	is the height of the zero-displacement plane (see below),
z_{0m}	$[m]$	is the roughness length controlling transfer of momentum, and
z_{0c}	$[m]$	is the roughness length controlling transfer of water vapour, carbon dioxide, and sensible heat (often taken to be the same as z_{0m}).

The zero-displacement height, z_d , can be estimated from the canopy height:

$$z_d = R_{dC} z_C \quad [m] \quad (19)$$

R_{dC}	$[-]$	ratio of the zero-displacement height to the canopy height ($0 \leq R_{dC} \leq 1$),
z_C	$[m]$	canopy height.

The roughness length controlling transfer of momentum, z_{0m} , is taken to be a fraction of the plant canopy height:

$$z_{0m} = R_{rC} z_C \quad [m] \quad (20)$$

R_{rC}	$[-]$	ratio of the roughness length controlling transfer of momentum to the canopy height ($0 \leq R_{rC} \leq 1$).
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As noted above, the roughness length controlling transfer of water vapour, carbon dioxide, and sensible heat, z_{0c} , is taken to be the same as the roughness length controlling transfer of momentum (Harman & Finnigan 2008, Kovalets et al. 2018):

$$z_{0c} = z_{0m} \quad [m] \quad (21)$$

¹³ Equation 5.7 of Hoch (2014).

The wind profile above and within a plant canopy, along with the relationship between the canopy height and the zero-displacement plane are illustrated in Fig. 3-2.

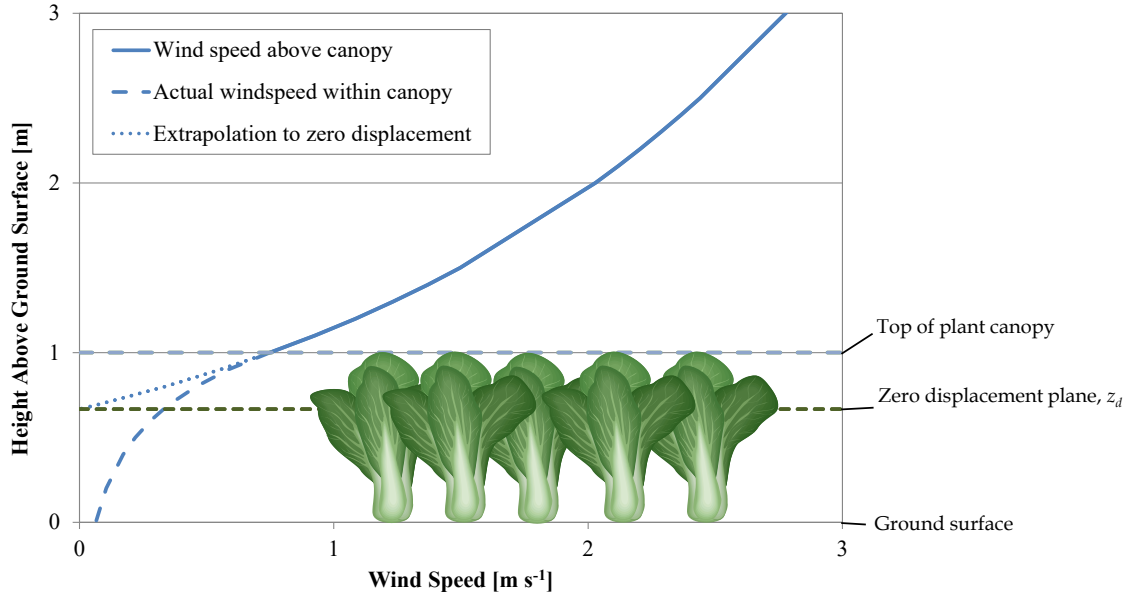


Fig. 3-2: Illustration of wind speed above and within a plant canopy, as well as the relationship between the plant canopy height, wind speed and the height of zero displacement
Adapted from Thorne & Walke (2013).

The relevant transport resistance $\Omega^{j,j+1}$ between the midpoints of layers j and $j+1$ is given by (based on Limer et al. 2011):

$$\Omega^{j,j+1} = \int_{\zeta - \frac{h^j}{2}}^{\zeta + \frac{h^{j+1}}{2}} \frac{dz}{D(z)} \quad [s \, m^{-1}] \quad (22)$$

Where ζ represents the position of the interface, and h is the vertical thickness of the layers.

If uniform diffusion/dispersion coefficients are employed in each layer one has:

$$\Omega^{j,j+1} = \frac{1}{2} \left(\frac{h^j}{D^j} + \frac{h^{j+1}}{D^{j+1}} \right) \quad [s \, m^{-1}] \quad (23)$$

The diffusive/dispersive transfer rate from compartment j to $j+1$, $\lambda_D^{j,j+1}$ is given by:

$$\lambda_D^{j,j+1} = \frac{1}{\Omega^{j,j+1} h_j} \quad [s^{-1}] \quad (24)$$

with a return transfer from layer $j+1$ to j :

$$\lambda_D^{j+1,j} = \frac{1}{\Omega^{j+1,j} h_{j+1}} \quad [s^{-1}] \quad (25)$$

The transfer rates require the effective diffusion/dispersion coefficients for the Topsoil Gas, Canopy Atmosphere and Top Atmosphere.

The effective diffusion coefficient for soil, D_{soil} , is a multiple, f_s , of the free air value, D_{air} :

$$D_{soil} = f_s D_{air} \quad [m^2 s^{-1}] \quad (26)$$

Typically, f_s , is less than 1.0 because it takes account of the effects of tortuosity in the gas-filled soil porosity, but it could be larger than 1.0 if turbulent mixing penetrated the soil to any significant degree.

The transport resistance across the full height of the canopy can also be written as:

$$\Omega^{Canopy} = \frac{z_C}{D_{Canopy}} \quad [s m^{-1}] \quad (27)$$

$$D_{Canopy} \quad [m^2 s^{-1}]$$

is the effective diffusion coefficient for the Canopy Atmosphere.

Which means that:

$$D_{Canopy} = \frac{z_C}{\Omega^{Canopy}} \quad [m^2 s^{-1}] \quad (28)$$

Finally, the diffusion/dispersion coefficient for the Top Atmosphere, is given by:

$$D_{AT} = D_{air} + k u^* (z_{Ref} - z_d) \quad [m^2 s^{-1}] \quad (29)$$

$$u^* \quad [m s^{-1}]$$

friction velocity that depends on the wind speed away from the surface and the surface roughness length, which is in turn related to the height of the roughness elements (here the plant canopy).

This provides the basis for calculating the exchanges of stable carbon between the Topsoil Gas, Canopy Atmosphere and Top Atmosphere¹⁴:

$$FC_{j,j+1} = \lambda_D^{j,j+1} AC_j \quad [kg_C a^{-1}] \quad (30)$$

j index for compartment Topsoil Gas or Canopy Atmosphere,
 $j+1$ successor of j in the sequence Topsoil Gas, Canopy Atmosphere and Top Atmosphere.

The diffusive/dispersive flux from the Top Atmosphere to the Wider Atmosphere need not be explicitly calculated, as the loss from the compartment is determined by the carbon balance (see Fig. 3-1).

For completeness, a diffusive flux of stable carbon from the Wider Atmosphere to the Top Atmosphere is needed. This is not a very important consideration because the advective flux is so large that, for any reasonable area, the activity diffusing into the atmosphere above the top layer will be almost entirely swept out of the model domain. Nonetheless, a diffusive flux can be defined if it is assumed that the wider atmosphere has the same dimensions as the top layer. The amount of stable carbon in the layer of the atmosphere involved in the diffusive exchange with the top layer is therefore the same as the amount within the air above, $AC_{AW} = AC_{AT}$. Consistent with Equation 20, the transport resistance can be defined as:

$$\Omega^{AW,AT} = \frac{1}{2} \left(\frac{h^{AT}}{D^{AT}} + \frac{h^{AT}}{D^{AT}} \right) = \frac{h^{AT}}{D^{AT}} \quad [s m^{-1}] \quad (31)$$

The total stable carbon flux from the Wider Atmosphere to Top Atmosphere, FC_{AW_AT} , has two components: (i) advective flow of carbon from up-wind and (ii) diffusion from the wider atmosphere. The stable carbon flux from the Wider Atmosphere to the Top Atmosphere is given by:

$$FC_{AW_AT} = u_{AT} W_f h_{AT} f_{CO2} C_{fCO2} + \lambda_D^{AW,AT} AC_{AW} \quad [kg_C a^{-1}] \quad (32)$$

u_{AT} $[m a^{-1}]$ representative wind speed for the Top Atmosphere,
 W_f $[m]$ width of the field,
 h_{AT} $[m]$ thickness of the top layer,
 $\lambda_D^{AW,AT}$ $[a^{-1}]$ transfer rate due to diffusion from the Wider Atmosphere (based on Equations 22 and 24).

The wind speed at the mid-point of the top layer is taken to be the appropriate representative value. Although this assumes a linear rather than a logarithmic wind profile, it is a minor consideration (see below).

Above a plant canopy the wind speed demonstrates a logarithmic wind profile, whilst within a plant canopy there is an exponential decrease in wind speed (Foken 2008). Details of the exponential decrease within the canopy can be ignored on the basis that it will have relatively

¹⁴ Note that conversion between units of time from s^{-1} to a^{-1} is implicitly assumed.

little impact on the wind speed at the mid-point of the turbulent layer, given the 10 m height of the top layer in relation to the height of crops and pasture. The wind speed can instead be calculated directly from a logarithmic wind profile where the wind speed at 10 m, U_{10} , m s^{-1} , is an input and the wind speed is taken to reduce to zero at z_d from¹⁵:

$$u(z) = u_{10} \frac{\ln(z/z_d)}{\ln(z_{10}/z_d)} \quad [\text{m s}^{-1}] \quad (33)$$

where z is the height at which the wind speed is required and z_{10} is the 10 m height. This function is illustrated in Fig. 3-2 assuming u_{10} of 5 m s^{-1} , a canopy height of 1 m and z_d to be 2/3 of the canopy height.

Assuming a uniform wind rose, the width of the field, W_f , is taken as being:

$$W_f = 2 \left(\frac{A_f}{\pi} \right)^{\frac{1}{2}} \quad [\text{m}] \quad (34)$$

The stable carbon flux from the Canopy Atmosphere to Above Ground Plant, FC_{AirPA} , is given by:

$$FC_{AP_PA} = Y_{G,PA} A_f C f_{OM} (1 - f_{CS,PA}) + Y_{G,PR} A_f C f_{OM} (1 - f_{CS,PR}) \quad [\text{kg C a}^{-1}] \quad (35)$$

$Y_{G,PA}, Y_{G,PR} \quad [\text{kg m}^2 \text{ a}^{-1}]$ gross dry weight annual assimilation of above-ground plants and roots,
 $f_{CS,PA}, f_{CS,PR} \quad [-]$ fraction of carbon in Above Ground Plant or Root derived from the soil.

The gross annual assimilation, Y_G , is given by:

$$Y_{G,i} = \frac{Y_{N,i}}{1 - f_R} \quad [\text{kg m}^{-2} \text{ a}^{-1}] \quad (36)$$

i compartment index for the Above Ground Plant (PA) or Plant Roots (PR),
 $Y_N \quad [\text{kg m}^2 \text{ a}^{-1}]$ net dry weight production of organic matter per year,
 $f_R \quad [-]$ respiration fraction of gross assimilation.

¹⁵ Note that conversion between units of time from s^{-1} to a^{-1} is implicitly assumed.

The net dry weight production of organic matter Y_N is derived from the component of the plant that is harvested and is given by:

$$Y_{N,i} = \frac{Y_{DW,i}}{f_H} \quad [kg\ m^2\ a^{-1}] \quad (37)$$

i compartment index for the Above Ground Plant (PA) or Plant Roots (PR),
 Y_{DW} $[kg\ m^2\ a^{-1}]$ dry weight yield of harvested crop,
 f_H $[-]$ fraction of the plant that is harvested above- or below-ground plant.

If the harvested component is above-ground, then the net production of organic matter for the below-ground plant is given by:

$$Y_{N,PR} = R_{RS} Y_{N,PA} \quad [kg\ m^2\ a^{-1}] \quad (38)$$

R_{RS} $[-]$ the dry weight root:shoot ratio.

If the harvested component is below-ground, then the net production of organic matter for the above ground plant, is given by:

$$Y_{N,PA} = \frac{Y_{N,PR}}{R_{RS}} \quad [kg\ m^2\ a^{-1}] \quad (39)$$

The dry weight yield of harvested crop is given by:

$$Y_{DW} = Y_{FW}(1 - f_w) \quad [kg\ m^2\ a^{-1}] \quad (40)$$

Y_{FW} $[kg\ m^2\ a^{-1}]$ fresh weight yield of harvested material,
 f_w $[-]$ fractional water content of the harvested material.

The stable carbon flux from Above Ground Plant to the Canopy Atmosphere due to plant respiration, FC_{PA_AL} , is given by:

$$FC_{PA_AP} = Y_{G,PA} f_{R,PA} A_f C f_{OM} \quad [kg_C\ a^{-1}] \quad (41)$$

The stable carbon flux from Topsoil Solution to Above Ground Plant, FC_{TS_PA} , is given by:

$$FC_{TS_PA} = Y_{G,PA} A_f C f_{OM} f_{CS,PA} + Y_{G,PR} A_f C f_{OM} f_{CS,PR} \quad [kg_C\ a^{-1}] \quad (42)$$

The stable carbon flux from Roots to Topsoil Solution, FC_{PR_TS} , is given by:

$$FC_{PR_TS} = A_f Y_{G,PR} f_{R,PR} C f_{OM} \quad [kg_C\ a^{-1}] \quad (43)$$

The stable carbon flux from Above Ground Plant to Roots, FC_{PA_PR} , is given by:

$$FC_{PA_PR} = Y_{G,PR} A_f C f_{OM} \quad [kg_C a^{-1}] \quad (44)$$

The stable carbon flux from Above Ground Plant to Elsewhere, FC_{PA_EW} , reflects the loss of carbon with harvested above-ground plant material and is given by:

$$FC_{PA_EW} = A_f Y_{N,PA} f_{H,PA} C f_{OM} = A_f Y_{DW,PA} C f_{OM} \quad [kg_C a^{-1}] \quad (45)$$

The stable carbon flux from Roots to Elsewhere, FC_{PR_EW} , reflects the loss of carbon with harvested below-ground plant material and is given by:

$$FC_{PR_EW} = A_f Y_{N,PR} f_{H,PR} C f_{OM} = A_f Y_{DW,PR} C f_{OM} \quad [kg_C a^{-1}] \quad (46)$$

The stable carbon flux from Above Ground Plant to Topsoil Organic Matter, FC_{PA_TO} , is given by:

$$FC_{PA_TO} = Y_{N,PA} A_f C f_{OM} (1 - f_{H,PA}) \quad [kg_C a^{-1}] \quad (47)$$

The stable carbon flux from Roots to Topsoil Organic Matter, FC_{PR_TO} , is given by:

$$FC_{PR_TO} = Y_{N,PR} A_f C f_{OM} (1 - f_{H,PR}) \quad [kg_C a^{-1}] \quad (48)$$

The following stable carbon fluxes (Eq. 46 – 50) are calculated by mass balance. The stable carbon flux from Topsoil Organic Matter to Topsoil Solution, FC_{TO_TS} , is given by:

$$FC_{TO_TS} = FC_{PR_TO} + FC_{PA_TO} \quad [kg_C a^{-1}] \quad (49)$$

The stable carbon flux from Topsoil Solution to Topsoil Gas, FC_{TS_TG} , is given by¹⁶:

$$FC_{TS_TG} = FC_{AW_TS} + FC_{LA_TS} + FC_{DS_TS} + FC_{TO_TS} + FC_{PR_TS} + FC_{WS_TS} - FC_{TS_DS} - FC_{TS_PA} \quad [kg_C a^{-1}] \quad (50)$$

Note that this treats the flux from solution to soil gas as one way. In practice, it will be rapidly bi-directional, so the model is calculating the net flux released to the soil gas. Whilst this means that carbon in the soil solution and soil gas could, in principle, be treated as a single compartment, it is considered conceptually useful to maintain a distinction.

¹⁶ FC_{TS_TG} should be greater than or equal to zero; if that is not the case, then it implies that there is an error in the model parameterisation that should be addressed.

The stable carbon flux from Topsoil Gas to Canopy Atmosphere, FC_{TG_AP} , is given by:

$$FC_{TG_AP} = FC_{TS_TG} + FC_{AP_TG} \quad [kg_C a^{-1}] \quad (51)$$

The stable carbon flux from the Canopy Atmosphere to the Top Atmosphere, FC_{AP_AT} , is given by:

$$FC_{AP_AT} = FC_{TG_AP} + FC_{PA_AP} + FC_{LA_AP} + FC_{WS_AP} - FC_{AP_TG} - FC_{AP_PA} \quad [kg_C a^{-1}] \quad (52)$$

The stable carbon flux from the Top Atmosphere to the atmosphere elsewhere, FC_{AT_AW} , is given by:

$$FC_{AT_AW} = FC_{AP_AT} + FC_{AW_AT} - FC_{AT_AP} \quad [kg_C a^{-1}] \quad (53)$$

3.4 C-14 transfer model

A source flux, SF_{LA} , equivalent to 1 Bq kg_C^{-1} of C-14 in contaminated groundwater from the geosphere is introduced to the Local Aquifer according to:

$$SF_{LA} = C_{GW} F_{SC,LA} C_{fW,LA} \quad [Bq a^{-1}] \quad (54)$$

C_{GW} $[Bq kg_C^{-1}]$ specific activity of C-14 in the contaminated groundwater, i.e. 1 Bq kg_C^{-1} ,

$F_{SC,LA}$ $[m^3 a^{-1}]$ flux of contaminated groundwater into the local aquifer.

The C-14 is then transferred around the model according to:

$$\lambda_{C-14,ij} = \frac{FC_{ij}}{AC_i} \quad [a^{-1}] \quad (55)$$

$\lambda_{C-14,ij}$ $[a^{-1}]$ transfer rate for C-14 from compartment i to j ,

FC_{ij} $[kg_C a^{-1}]$ flux of stable carbon,

AC_i $[kg_C]$ amount of stable carbon in the donor compartment.

Specific activities, SpA , can be calculated for the modelled compartments according to:

$$SpA = \frac{N}{AC} \quad [Bq kg_C^{-1}] \quad (56)$$

N $[Bq]$ amount of C-14 in a compartment.

3.5 SwiBAC parameters

The behaviour of C-14 represented by the C-14 model needs to be replicated in Nagra's generic biosphere model SwiBAC for assessing the exposure of humans by radionuclides released from the repository to the biosphere. This can be done by considering the way in which the C-14 model relates to the SwiBAC model.

The C-14 model includes compartments for the representation of the crop plant and the atmosphere that do not exist in the SwiBAC dynamic transport model. Moreover, losses from surface water and topsoil to atmosphere and harvesting of the crop result in additional losses of C-14 from the system.

Including in SwiBAC additional loss terms for C-14 from the surface water and topsoil compartments, allows these losses to be taken into account. Furthermore, adjusting the effective distribution of C-14 between solid and liquid phases in the SwiBAC compartments Topsoil, Deep Soil, Variably Saturated Zone and Local Aquifer allows the transfer rates of C-14 between these compartments to approximate the corresponding transfer rates of the C-14 model. The uptake of C-14 by plants can be represented in SwiBAC using a soil-to-plant concentration ratio calculated with the C-14 model.

The derivation of the additional loss terms, the effective distribution between solid and liquid phases and the soil-to-plant concentration ratios are described in detail in the sub-sections below. Furthermore, the impact of the (wrt. to SwiBAC) additional transboundary fluxes for harvest and degassing on interfacing the dynamic transport model with the exposure model in SwiBAC is discussed.

3.5.1 Additional loss term from the surface soil

The net flux of C-14 from the topsoil other than that mediated by advection with water reflects an additional loss term that needs to be introduced into the SwiBAC model. This represents C-14 that is lost to the atmosphere and that is lost in harvested plant material. If the total transfer flux of C-14 from compartment i to compartment j is represented as TF_{ij} , then the net flux from the topsoil, TF_{soil} , is given by:

$$TF_{soil} = TF_{TG,AP} + TF_{TS,PA} - TF_{AP,TG} - TF_{PR,TS} - TF_{PR,TO} - TF_{PA,TO} \quad [Bq\ a^{-1}] \quad (57)$$

$$TF_{ij} \quad [Bq\ a^{-1}] \quad \text{total transfer flux of C-14 from compartment } i \text{ to } j.$$

This can be converted into a net loss rate, λ_{soil} , by comparison with the amount of C-14 in the topsoil:

$$\lambda_{soil} = \frac{TF_{soil}}{N_{TS} + N_{TO} + N_{TG}} \quad [a^{-1}] \quad (58)$$

$$N_i \quad [Bq] \quad \text{calculated amount of C-14 in compartment } i \text{ at steady state.}$$

3.5.2 Effective distribution between solid and liquid phases

In both SwiBAC and the C-14 model, transfers between the topsoil, deep soil, variably saturated zone and local aquifer are mediated by water flux. In SwiBAC, the rates for these transfers are determined by the rate of water flux, the water-filled porosity and the capacity of the compartments for retention on the solid phase (neglecting transport by suspended solids and diffusion):

$$\lambda_{ij} = \frac{F_{ij}}{(\theta_{w,i} + \rho_{b,i} K_{d,i}) V_i} \quad [a^{-1}] \quad (59)$$

Within the C-14 model, the rates for these transfers are based on Equations 2, 12 and 56, such that the transfer rate is given by:

$$\lambda_{ij} = \frac{F_{ij} C f_{w,i}}{f_{EC} f_{CC,i} C f_{CC} V_i \rho_{b,i}} \quad [a^{-1}] \quad (60)$$

The rates for these transfers in the C-14 model can be replicated in SwiBAC by calculating effective K_d values by rearranging Equation 61:

$$K_{d,i} = \frac{F_{ij} - \theta_{w,i} \lambda_{ij} V_i}{\lambda_{ij} \rho_{b,i} V_i} \quad [m^3 kg^{-1}] \quad (61)$$

Substituting Equation 62 into Equation 63, the flow rates and volumes cancel out, such that the effective K_d values can be calculated using:

$$K_{d,i} = \frac{f_{EC} f_{CC,i} C f_{CC}}{C f_{w,i}} - \frac{\theta_{w,i}}{\rho_{b,i}} \quad [m^3 kg^{-1}] \quad (62)$$

The second term will be relatively small for the deep soil, variably saturated zone and aquifer compartments, therefore this effectively becomes:

$$K_{d,i} = \frac{f_{EC} f_{CC,i} C f_{CC}}{C f_{w,i}} \quad [m^3 kg^{-1}] \quad (63)$$

i compartment index *DS* or *LA*.

This expression provides a means of calculating the K_d value for the deep soil, variably saturated zone and aquifer compartments in SwiBAC, which are each represented with a single compartment in both models. However, for the SwiBAC topsoil compartment, it has to be considered that transfer rates relate to the amount of C-14 of three compartments of the C-14 model. In order to keep the flux of C-14 from the topsoil to the deep soil conceptually invariant

for both models the transfer rate $\lambda_{TS,DS}$ relating to Topsoil Solution has to be re-scaled to $\lambda_{T,D}$ relating to the total Topsoil.

$$\lambda_{T,D} = \frac{N_{TS}}{N_{TS} + N_{TO} + N_{TG}} \lambda_{TS,DS} \quad [a^{-1}] \quad (64)$$

N_i $[Bq]$ calculated amount of C-14 in compartment i at steady state.

The distribution coefficient between the solid and liquid phase for topsoil effectively becomes:

$$K_{d,T} = \frac{N_{TS} + N_{TO} + N_{TG}}{N_{TS}} \frac{f_{EC} f_{CC,TS} C f_{CC}}{C f_{W,TS}} \quad [m^3 \text{ kg}^{-1}] \quad (65)$$

3.5.3 Soil-to-plant concentration ratio

The soil-to-plant concentration ratio can be calculated from the C-14 concentration in the fresh plant and the C-14 concentration in the dry soil. The fresh plant biomass can be derived from the dry biomass, B , according to $B/(1-f_w)$. The fresh weight related activity concentration of C-14 in the above-ground plant, C_{PA} , is therefore calculated given by:

$$C_{PA} = \frac{N_{PA}(1 - f_w)}{A_f B_{PA}} \quad [Bq \text{ kg}_{\text{fresh}}^{-1}] \quad (66)$$

Similarly, the concentration in the roots per fresh weight, C_{PR} , is given by:

$$C_{PR} = \frac{N_{PR}(1 - f_w)}{A_f B_{PR}} \quad [Bq \text{ kg}_{\text{fresh}}^{-1}] \quad (67)$$

The activity concentration in topsoil per dry weight, C_T , is given by:

$$C_T = \frac{N_{TS} + N_{TO} + N_{TG}}{V_T \rho_{b,T}} \quad [Bq \text{ kg}_{\text{dry}}^{-1}] \quad (68)$$

The effective soil-to-plant concentration ratio, CR , is given below, with the use of C_{PA} or C_{PR} being determined by whether the harvested component is above- or below-ground.

$$CR = \frac{C_{PA}}{C_T} \quad \text{or} \quad CR = \frac{C_{PR}}{C_T} \quad \left[\frac{Bq \text{ kg}_{\text{fresh}}^{-1}}{Bq \text{ kg}_{\text{dry}}^{-1}} \right] \quad (69)$$

3.5.4 Interfacing the dynamic transport model and the exposure model

The SwiBAC biosphere assessment model simulates the migration and distribution of radionuclides (referred to as transport) released from a deep geological repository to an agricultural biosphere system and evaluates potential exposure of humans based on the resulting distribution of radionuclides, i.e. the radionuclide concentration in the compartments Topsoil, Surface Water and Local Aquifer.

Originally, the only possible losses of radionuclides from the system were the out-fluxes of radionuclides from the compartments Surface Water and Local Aquifer as well as radioactive decay. Pathways of ingestion via harvest of crops, use of animal products and drinking water as well as the pathway of inhalation via degassing from soil are taken into account - but without impact on the distribution of radionuclides in the system.

Fluxes of C-14 out of the system due to harvest and degassing have to be considered in SwiBAC (by introducing the additional loss terms) in order to make the distribution of C-14 in SwiBAC match the distribution of the radionuclide in the C-14 model. These fluxes can result in an exposure of humans by ingestion or inhalation. Ingestion via harvest is modelled in SwiBAC by deriving concentrations in crops from the concentration in soil (applying transfer factors) and assuming rates for yield and consumption of crop; inhalation via degassing is considered by a breathing rate and a radionuclide concentration in air derived from its concentration in soil by means of a degassing rate¹⁷. These pathways are parameterised in such a way that the corresponding fluxes match the fluxes calculated from the C-14 model. Degassing from surface water is taken to have a negligible effect on inhalation exposure due to the significant degree of dispersion that would arise.

¹⁷ Details are to be found in (Nagra 2024b).

4 Parameter values

4.1 Biosphere- and climate-dependent parameters

Some parameters depend on the biosphere system and climate being modelled. These parameters are listed in Tab. 4-1 and the values are based on those as given in Nagra (2014). Note that the use of crop-independent water fluxes in the C-14 model means that there is an assumption that all crops modelled are grown in soil subject to the same rate of irrigation.

Tab. 4-1: System-dependent parameters

Parameter		Description
V	$[m^3]$	The volume of the compartment
θ_t	$[-]$	The total porosity of the compartment
θ_w	$[-]$	The volumetric moisture content of the compartment
ρ_g	$[kg\ m^{-3}]$	The grain density of solid material in the compartment
A_f	$[m^2]$	The area of the agricultural land
A_{WS}	$[m^2]$	The area of the surface water
F	$[m^3\ a^{-1}]$	The appropriate water flux
$d_{precipit}$	$[m\ a^{-1}]$	The precipitation rate

4.2 Crop-independent parameters

The required crop-independent parameters are given in Tab. 4-2. Short notes are included in the table, whilst longer discussions are numbered and described below.

- A. Sheppard et al. (2006) discuss the different forms of carbon in plants and their carbon content and give values between 42% and 77% carbon by dry weight in the individual plant components. Soil organic matter as well as all plant organic matter is assumed to contain a down-rounded value of 40% C by weight ($C_nH_{2n}O_n$ assumed).
- B. The inorganic carbon content in water depends on many factors (see e.g. Kirby and Cravotta III 2005a,b). It is difficult to measure and the measured data are also difficult to interpret. In Davis et al. (1993) a range of 0.02 to 0.068 kg m⁻³ water is reported with a triangular distribution and a peak value of 0.04 kg m⁻³ water. Thorne (2005b) assumed values ranging from 0.001 to 0.01 kg m⁻³. Measurements in the deep groundwater in the borehole in Benken (Switzerland) produced values between 0.05 and 0.1 kg m⁻³ Nagra (2001).

In the current model all water is assumed to have the same constant concentration of inorganic carbon. The carbon content in all groundwater is assumed to be 0.04 kg m⁻³ water, chosen as intermediate value within the range previously listed.

- C. The concentration of CO₂ in the soil atmosphere is expected to be enriched by a factor of between 10 to 60 in comparison to the above-ground atmosphere (see, e.g., Suarez & Šimůnek 1993). A reference value of 30 is adopted, as a mid-point value.

Tab. 4-2: Crop-independent parameters

Representative of present-day conditions, consistent with reference biosphere modelling in Nagra (2024b). These are taken to be suitably representative of the range of conditions considered in biosphere modelling.

Parameter		Description	Value	Notes
Cf_{CC}	$[-]$	Mass fraction of carbon in calcium carbonate	0.12	Based on CaCO_3
Cf_{CO_2}	$[\text{kg}_C \text{m}^{-3}]$	Mass of inorganic carbon in 1 m ³ of CO_2	$\frac{12 \text{ g}_C}{22.4 \text{ L}}$	1 mol CO_2 occupying 22.4 L at standard temperature and pressure.
Cf_{OM}	$[-]$	Mass fraction of carbon in organic matter	0.4	A
Cf_P	$[\text{kg}_C \text{m}^{-3}]$	Carbon content in precipitation	0.04	Taken to be the same as Cf_W
Cf_W	$[\text{kg}_C \text{m}^{-3}]$	Carbon content in the appropriate water	0.04	B
E_f	$[-]$	Enhancement factor for the concentration of stable carbon in the soil gas in comparison to the canopy atmosphere	30	C
f_{CC}	$[-]$	Mass fraction of the compartment solid as calcium carbonate	0.05	D
f_{CO_2}	$[-]$	Volumetric fraction of CO_2 in the air above the canopy	0.0004	E
f_{CS}	$[-]$	Fraction of root or above-ground plant carbon derived from the soil	0.02	F
f_{degass}	$[-]$	Fraction of carbon content in irrigation water lost to the atmosphere due to degassing	0	Conservative modelling assumption
f_{EC}	$[-]$	Exchangeable carbonate as a mass fraction of the total carbonate	0.1	D
f_{OM}	$[-]$	Organic matter content of the topsoil solid as a mass fraction	0.05	G
f_R	$[-]$	Respiration fraction of gross organic matter assimilation by plants	1/3	H
f_s	$[-]$	Ratio of the diffusion coefficient in soil to that in free air	0.1	I
k	$[-]$	von Kármán's constant	0.41	J
u^*	$[\text{m s}^{-1}]$	Friction velocity	0.35	K
R_{dC}	$[-]$	Ratio of the zero displacement height to that of the top of the canopy of the dominant plant species	2/3	L
R_{rC}	$[-]$	Ratio of the roughness length controlling transfer of momentum to the canopy height of the dominant plant species	0.1	M
D_{air}	$[\text{m}^2 \text{s}^{-1}]$	Molecular diffusion coefficient in free air	1.4E-5	N
u_0	$[\text{m s}^{-1}]$	Wind speed at 10 m height above ground	5	O

- D. The model includes compartments for soil organic matter and CO_2 / bicarbonate in solution and rates of exchange are calculated assuming steady state. The exchange of inorganic carbon between the water and solid carbonate can be represented as a distribution between solid and liquid phases and modelled with a K_d . As discussed in Brennwald & van Dorp (2008), Nagra's biosphere modelling for Project Opalinus Clay used a K_d value for C-14 of 5 L kg⁻¹ based on the assumption that the soil contains 5% carbonate (by dry weight) of which only 1% is available for exchange. Sheppard et al. (1998) indicate a K_d for a soil containing 6% CO_3^{2-} (10% CaCO_3) of 30 L kg⁻¹. Sheppard et al. (1990) report soil K_d values based on a specific activity model of between 0.3 and 7 L kg⁻¹ with a geometric mean of 1.2 for C-14 and values of 9 and 80 L kg⁻¹ for stable carbon. The reported experiments indicate that a large fraction of the CaCO_3 is involved in the exchange between water and solid phase. The long timescales over which radionuclides from deep geological repositories would enter the biosphere would lead to a large fraction of CaCO_3 in the soil being exchangeable. Kuzyakov et al. (2006) report models and measurements concerning the effects of root respiration and the decomposition of soil organic matter on dissolution and re-crystallization of calcium carbonate in loess soils. According to that paper, complete (99%) recrystallization of calcium carbonate would require between 100 and 2'000 years. The model presented here assumes 5% (weight) calcium carbonate in the top and deep soil and 5% in the biosphere aquifer; 10% of this carbonate is assumed to be involved in the exchange between solid and water (which seems to be a low value compared with the data in the cited references). As mentioned above, this carbonate has no influence on the steady state fluxes through the biosphere but determines the time required to reach steady state.
- E. The volumetric fraction of CO_2 is taken to be 400 ppmv, which is slightly lower than present day value (412 ppmv), and much lower than values likely to occur over the next few hundred years depending on the fossil carbon emissions scenario assumed.
- F. The major part of carbon in terrestrial plant material is derived from atmospheric carbon dioxide (Sheppard & Thorne 2005). A small fraction, however, might be derived from inorganic carbon in soil. Sheppard et al. (1990) report soil to plant transfer factors for C-14 derived from soil of 0.015 to 2.3 (Bq kg⁻¹ dry plant)/(Bq kg⁻¹ dry soil). They calculated that 0.002% (in an acidic soil) to 1.4% (in a carbonate soil) of the plant carbon was derived from the soil. Vuorinen et al. (1989) and Amiro & Ewing (1992) report experimental results and literature values in the range of 1% to 2%. For the present calculations it is assumed that 2% of the gross production of organic plant material (above-ground and roots) is derived from inorganic carbon in the soil water (this is pessimistic, because it is at the top end of the range).
- G. A mass fraction of 5% is assumed for the organic matter content in the soil, which is assumed to be constant over time.
- H. Van Keulen & Wolf (1986) and Penning de Vries (1975) report that respiration for maintenance can be between 0.01 and 0.03 kg kg⁻¹ d⁻¹ and the carbon required in respiration to transform organic compounds within the plant into others is 0.3 to 0.75 kg kg⁻¹. The present model assumes that 1/3 is lost by respiration both of the gross production to the atmosphere for the above-ground plant parts and to the soil for the roots.
- I. The effective diffusion coefficient of CO_2 in soil has been extensively studied (see, for example, De Sutter et al. 2008). The diffusion coefficient D_{soil} is a fraction f_s of the free air value, D_{air} , of approximately $1.4 \cdot 10^{-5} \text{ m}^2 \text{ s}^{-1}$. For agricultural soils, Hoch (2014) estimated values of 0.025 to 0.22; a value of 0.1 is used here.
- J. Based on Zhang et al. (2008).
- K. Based on Thorne & Walke (2013), selecting a representative value between that for short grass (0.26 m s⁻¹) and the general value for agricultural areas (0.54 m s⁻¹).

- L. Allen et al. (1998) observed that for a wide range of crops the zero plane displacement height, z_d can be estimated by assuming that it is two-thirds of the canopy height. A study of a barley field in Estonia concluded that the calculated z_d could be taken as three-quarters and two-thirds of z_C for a dense and a moderate canopy, respectively (Mölder 1997). Amiro et al. (1991) give z_d as a sixth or tenth of the vegetation height, whilst Avila & Pröhl (2008) report heights for farmlands and forests, which are $\frac{1}{4}$ and $\frac{1}{2}$ of the vegetation height, respectively. A reference value of two-thirds is adopted here, consistent with Allen et al. (1998).
- M. Simple approximation given by Foken (2008).
- N. Based on Lide (2006).
- O. Value for neutral atmospheric stability conditions (Pasquill Category D), based on Clarke (1979). Neutral conditions represent an intermediate point between stable and unstable atmospheric conditions and are therefore considered representative of typical conditions.

4.3 Crop-dependent parameters

The crops considered in the model are cereals, root vegetables, green vegetables, fruit and animal feed (fodder), which reflect those represented in SwiBAC (Nagra 2024b). The animal feed is taken to represent a combination of grazed pasture, hay and fodder maize. A “generic” crop is also included for use in reference calculations and was useful in development of the model.

The required crop-dependent parameters are given in Tab. 4-3, with further notes given below. Note that the net dry weight production rates for the generic crop, $Y_{N,PA}$ and $Y_{N,PR}$, are specified directly, so the parameterisation differs from that of the other crops.

- A. The parameter values are adopted as reasonable modelling assumption.
- B. The water content of crops is taken from IAEA (2010).
- C. The fresh weight crop yields are consistent with Nagra (2024b) with small rounding differences.
- D. Assumption of net dry weight organic matter production rates of $2 \text{ kg m}^{-2} \text{ a}^{-1}$ for both the above-ground plant and roots is adopted for the generic crop.

Tab. 4-3: Crop-dependent parameters.
Notes on the adopted values are given in the text.

Parameter	Description and units		Values						Notes
			Generic Crop	Cereals	Root Vegetables	Green Vegetables	Fruit	Fodder	
f_H	Fraction of the plant that is harvested	Above-ground	0.5	0.5	0	0.8	0.5	0.8	A
		Below-ground	0.5	0	2/3	0	0	0	
f_w	Fractional water content of the harvested material, [-]		-	0.1	0.8	0.9	0.9	0.8	B
H_{AC}	Height of the plant canopy, [m]		1	1	0.5	0.5	0.5	0.5	A
R_{RS}	Dry weight root:shoot ratio, [-]		1	1	3/2	1/3	2/3	1	A
Y_{FW}	Fresh weight yield of harvested material, [kg m ⁻² a ⁻¹]		-	0.607	3.996	2.956	2.5	1.2	C
Y_N	Net dry weight production of organic material, [kg m ⁻² a ⁻¹]	Above-ground	2	-	-	-	-	-	D
		Below-ground	2	-	-	-	-	-	

5 Implementation

The model has been implemented in the AMBER generic compartment modelling software (Quintessa 2022). A screenshot is shown in Fig. 5-1. Data for the reference biosphere (based on present-day conditions) and alternative cases¹⁸ in Nagra (2024b) are included, together with data for the full range of crop types given in Section 4.3. The specific climate and crop type to be considered can be defined via drop-down “NameSet Option” parameters.

The model for C-14 draws on the water fluxes that form the basis of SwiBAC.

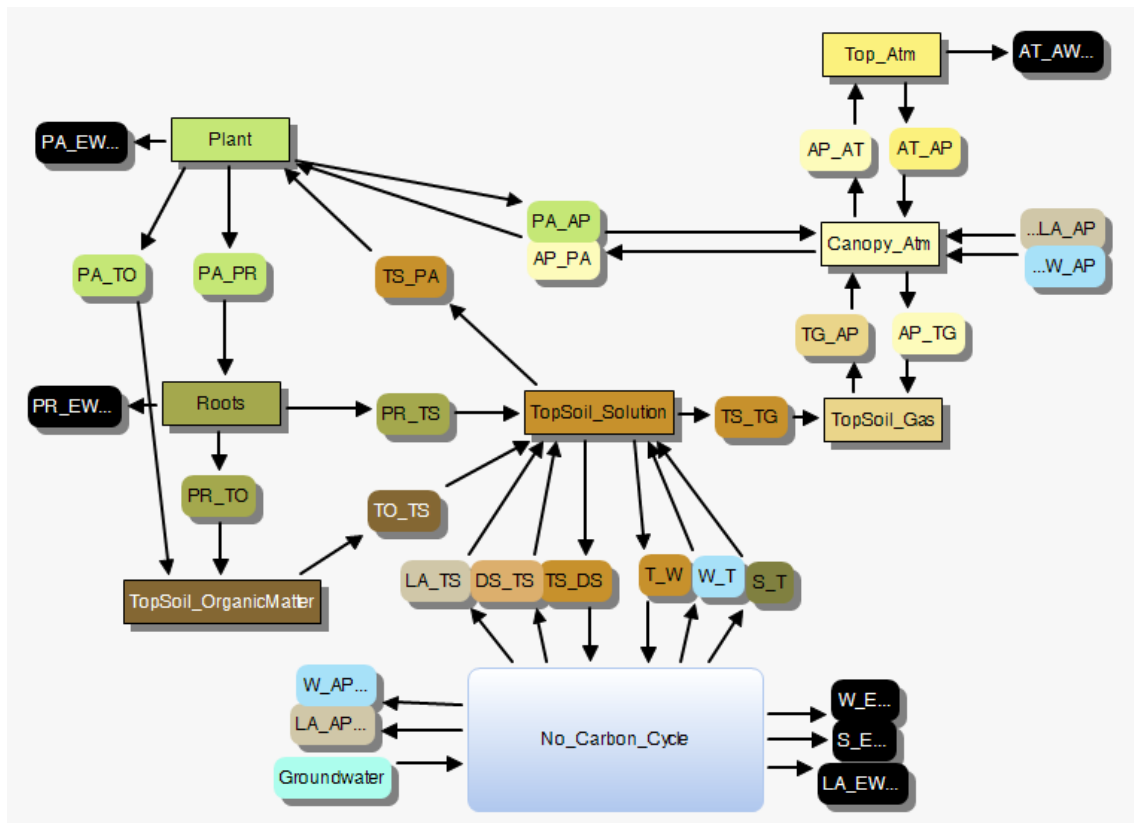


Fig. 5-1: Screenshot of the C-14 model implemented in AMBER

The model uses a precondition to check that the stable carbon fluxes into and out of each compartment as well as those into and out of the model domain balance. The precondition is set to produce an error if it fails, such that the model cannot be calculated if an error is introduced.

¹⁸ Alternative cases considered in Nagra (2024b) are: (i) a drained farmland case, (ii) a case with a warmer-drier climate, and (iii) a case based on cold climate conditions.

6 Illustrative calculations

An interaction matrix showing the stable carbon masses and balance for the reference biosphere with a generic crop is shown in Tab. 6-1. The table shows the relatively small amount of carbon within the soil gas, the canopy atmosphere and the top atmosphere compartments. The table also shows the dominance of the stable carbon flux through the top atmosphere.

The amount of C-14 in the model compartments for a unit source term of 1 Bq kgC^{-1} in contaminated groundwater discharge to the local aquifer is shown in Fig. 6-1 for the generic crop. The figure shows that it takes the system about 1'000 years to reach an equilibrium, which is determined by the relatively slow turnover rate of stable carbon in the local aquifer (Tab. 6-1 implies a characteristic time of retention within the local aquifer of about 460 years¹⁹). Retention within the variably saturated zone, deep soil and soil organic matter is sufficiently slow for their build up curves to differ from that of the local aquifer in Fig. 6-1. Turnover rates in other modelled compartments are relatively rapid (faster than once per year). Tab. 6-2 summarises amounts and fluxes of C-14 in the model for a generic crop at equilibrium.

Fig. 6-2 shows the resulting plant concentrations and associated specific activity for the generic crop, whilst Fig. 6-3 shows the effective soil-to-plant concentration ratios for different crops (Equation 71). The concentration ratios show an initial peak within the first five years before equilibrium is reached after about one hundred years.

The additional loss rate from the topsoil (Equation 60) is shown in Fig. 6-4 for the generic crop.

¹⁹ Tab. 6-1 shows $5.79\text{E}+7 \text{ kgC}$ in the Local Aquifer and a total loss rate of $1.28\text{E}+5 \text{ kgC a}^{-1}$. The amount divided by the loss rate gives a timescale of 460 years for an amount of carbon equivalent to the total amount of available carbon within the local aquifer to pass through. Mixing as the carbon passes through means that this reflects turnover rather than total replacement of available carbon within the local aquifer.

Tab. 6-1: Interaction matrix of stable carbon for the reference biosphere with a generic crop.

Stable carbon masses, $[kg_C]$, are given in the leading diagonal elements, stable carbon fluxes, $[kg_C a^{-1}]$, are given in the off-diagonal elements (interactions are illustrated in a clock-wise direction).

	Local aquifer	Variably sat. Zone	Deep soil	Surface water	Bed sediments	Topsoil solution	Topsoil gas	Canopy atmosphere	Top atmosphere	Above-ground plant	Below-ground plant	Topsoil organic matter	Elsewhere
Local aquifer	5.788E+07	0.000E+00			1.008E+05	2.730E+04		0.000E+00					0.000E+00
Variably sat. Zone	6.370E+04	8.681E+06	0.000E+00										
Deep soil		6.370E+04	4.341E+06			0.000E+00							
Surface water				4.550E+04	0.000E+00	0.000E+00		0.000E+00					4.681E+08
Bed sediments	0.000E+00			1.008E+05	7.000E+02								
Topsoil solution			6.370E+04			5.426E+05	2.675E+06			1.092E+05			
Topsoil gas							3.656E+02	2.848E+06					
Canopy atmosphere							1.723E+05	4.875E+02	8.544E+08	5.351E+06			
Top atmosphere								8.561E+08	4.388E+03				1.587E+09
Above-ground plant								9.100E+05		1.820E+06	2.730E+06	9.100E+05	9.100E+05
Below-ground plant						9.100E+05					1.820E+06	9.100E+05	9.100E+05
Topsoil organic matter						1.820E+06						1.809E+07	
Elsewhere	6.440E+04			4.680E+08		9.100E+04			1.589E+09				

Tab. 6-2: Amounts and fluxes of C-14 (for equilibrium conditions) for the reference biosphere with a generic crop

Unit source term (1 Bq kg^{-1}) of C-14 to the Local Aquifer; activities [Bq] are given in the leading diagonal elements, fluxes [Bq a^{-1}] are given in the off-diagonal elements (interactions are illustrated in a clock-wise direction).

[illegible]

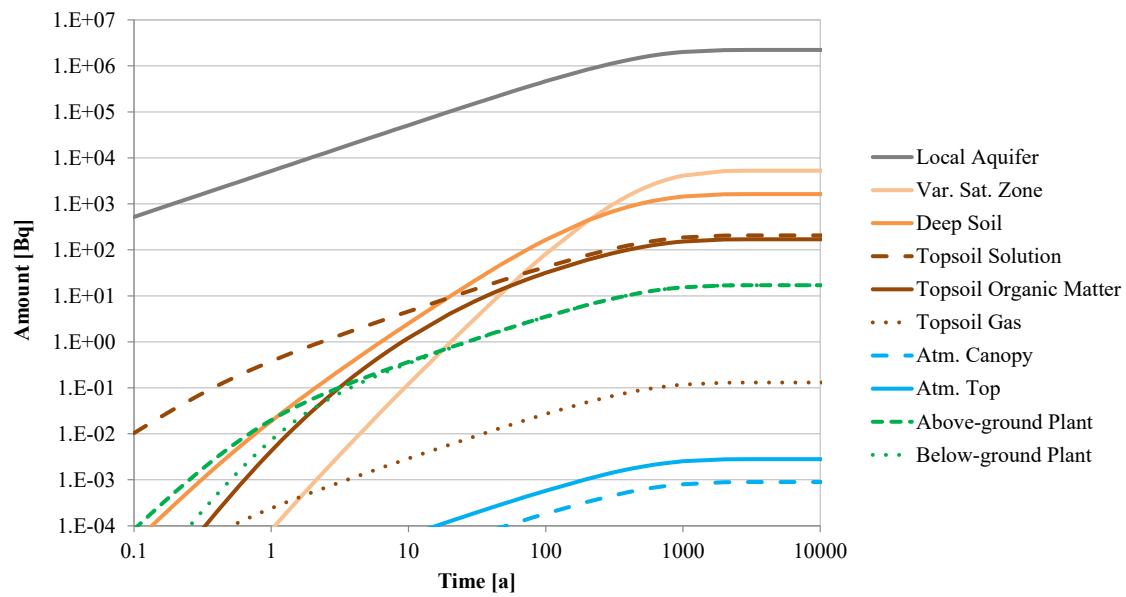


Fig. 6-1: Amount of C-14 in compartments for the reference biosphere
Amounts [Bq] are calculated for the generic crop with a unit source term (1 Bq/kg_C) in contaminated groundwater to the Local Aquifer.

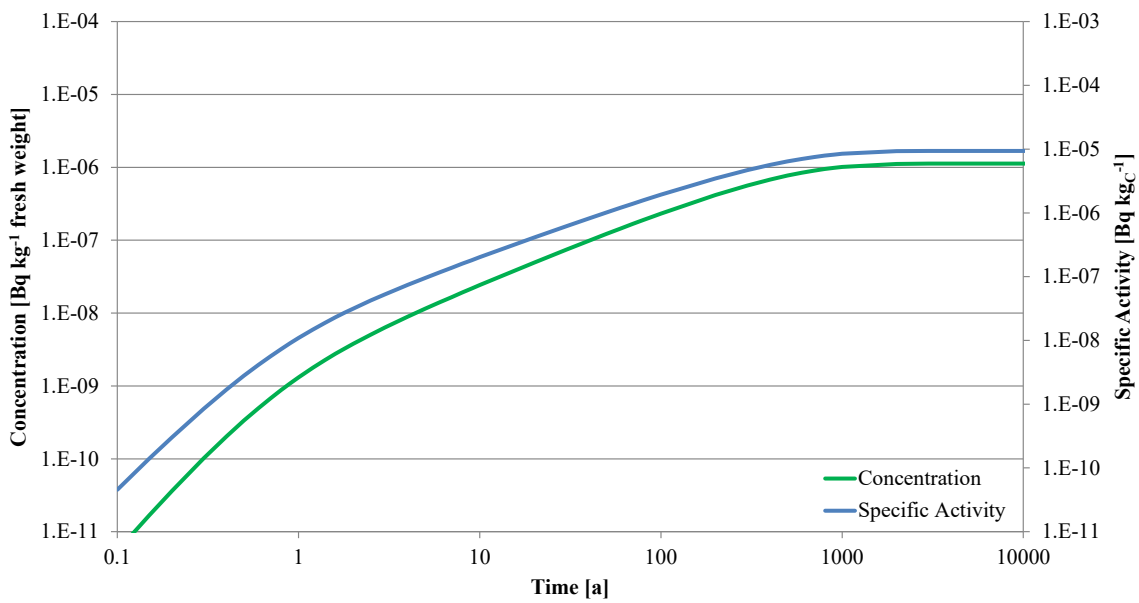


Fig. 6-2: Above-ground plant C-14 concentration and specific activity
Quantities are calculated for the generic crop and the reference biosphere with a unit source term (1 Bq/kg_C) in contaminated groundwater to the Local Aquifer.

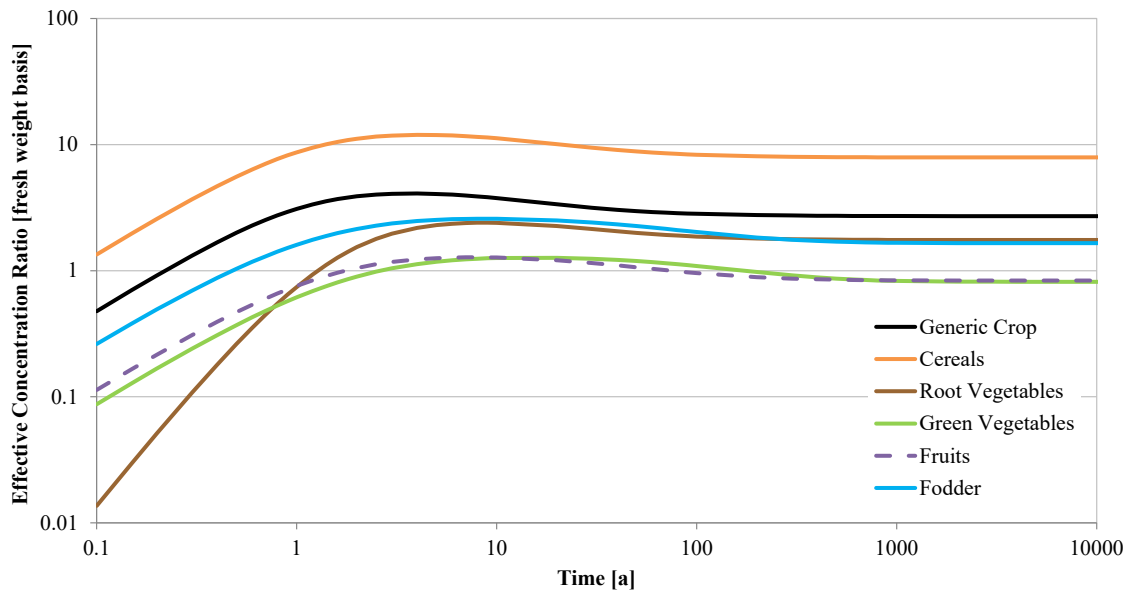


Fig. 6-3: Effective soil-to-plant concentration ratios for C-14 for the reference biosphere
Calculated with a unit source term (1 Bq/kg_C) in contaminated groundwater to the Local Aquifer.

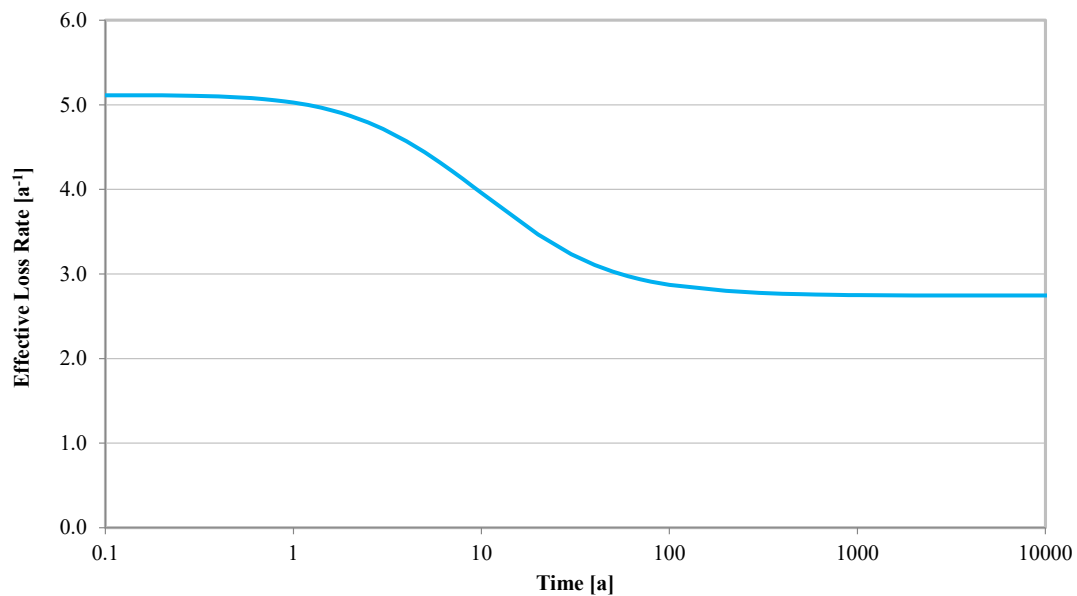


Fig. 6-4: C-14 loss rate from the topsoil for the reference biosphere with a generic crop
Calculated with a unit source term (1 Bq/kg_C) in contaminated groundwater to the local aquifer.

A key improvement to the modelling in comparison to Walke et al. (2013) has been to properly represent atmospheric mixing within the plant canopy atmosphere. Transfer rates for the transport of C-14 from the soil gas through to the above-canopy atmosphere are compared in Tab. 6-3. The comparison shows that rates of release from the soil gas are essentially the same as the previous model, but that there is a significantly higher degree of loss from the plant canopy atmosphere to the above-canopy atmosphere with the inclusion of turbulent mixing in the updated model, as expected. Rates of uptake from the canopy atmosphere to the plant are similar between the two models.

The effect of the improvement is to reduce the amount/concentration of C-14 in the plant canopy atmosphere. Fig. 6-5 compares the C-14 compartment amounts for the reference biosphere and generic crop between the new and previous models with a unit (1 Bq kg^{-1}) source to the local aquifer. The figure shows that the amounts of C-14 in the topsoil solution and above-canopy atmosphere are about the same between the previous and updated model, whereas the introduction of turbulent mixing in the plant canopy atmosphere reduces the amount of C-14 “seen” by the crop and results in less C-14 being taken up by the crop. This, in turn, results in less C-14 in topsoil organic matter when plant material that is not harvested becomes dead organic matter in the soil.

The reduction in the C-14 concentration in the plant canopy atmosphere means that less is taken up from the atmosphere by the plants. Indeed, Tab. 6-2 shows that the degree of dilution in the plant canopy atmosphere means that the 2% plant carbon that is modelled as being derived from root uptake of dissolved inorganic carbon dominates in terms of C-14 uptake by the plants (contributing 41 Bq a^{-1} to plant carbon given a unit source term to the local aquifer, compared to 10 Bq a^{-1} via uptake from the plant canopy atmosphere).

The effect of the improvements on parameter values calculated for representing C-14 in SwiBAC is explored in Section 7.

Tab. 6-3: Comparison of C-14 transfer rates (a^{-1}) from soil gas to the atmosphere above the crops, and the rate of uptake from the plant canopy atmosphere for the reference biosphere and a generic crop

Noting that Walke et al. (2013) modelled the lower atmosphere compartment as diffusively dominated to the zero displacement plane (typically 2/3 of canopy height) and included plant uptake from both the diffusive and turbulent layers, whereas the updated model represents the full canopy atmosphere with a single compartment that includes turbulent mixing.

Transfer	Walke et al. (2013)		Updated model
Soil gas to canopy atmosphere	7.69E+3		7.79E+3
Canopy atmosphere to top atmosphere	3.05E+3		1.75E+6
Canopy atmosphere to above-ground plant	Diffusive	8.64E+3	1.10E+4
	Turbulent	5.59E+2	

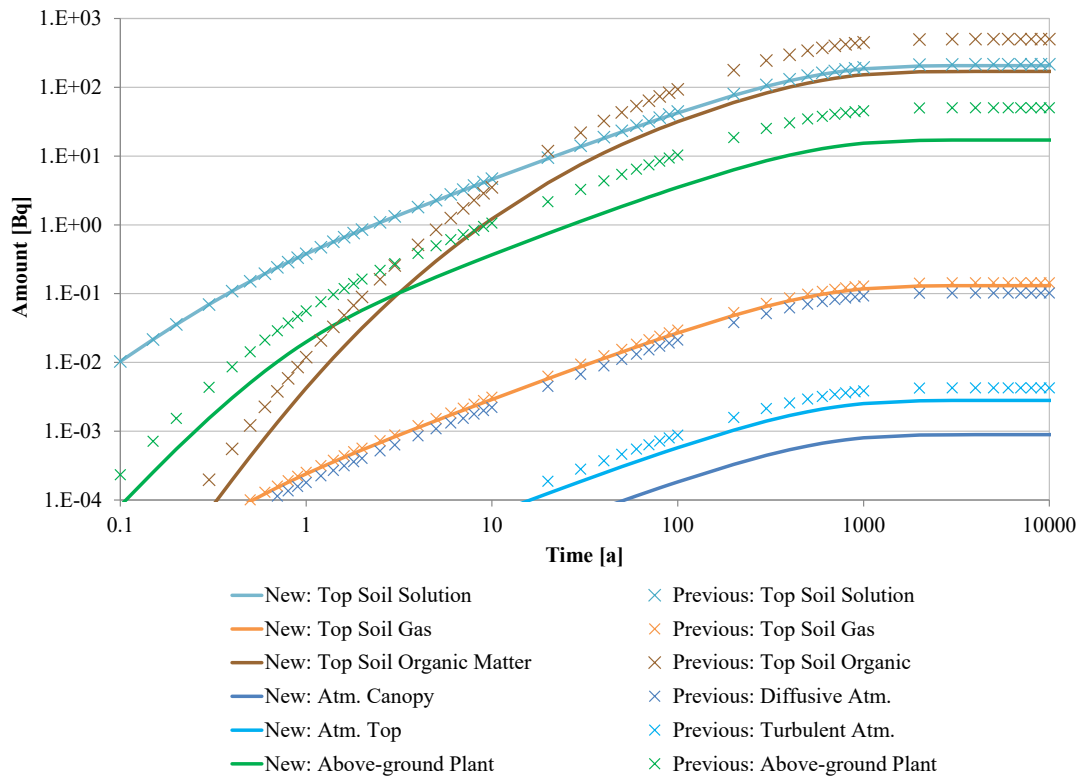


Fig. 6-5: Comparison of compartment amounts between the new and previous (Walke et al. 2013) biosphere model for C-14 for the reference biosphere with a generic crop. Calculated with a unit source term (1 Bq/kg_C) in contaminated groundwater to the local aquifer.

7 Integration within SwiBAC

Nagra's biosphere model for C-14, documented in Sections 2, 3 and 4, is used to calculate parameter values needed to adequately represent the behaviour of C-14 within Nagra's general biosphere modelling code, SwiBAC (Nagra 2024b), as discussed in Section 3.5.

Section 7.1 presents the SwiBAC parameter values calculated with the biosphere model for C-14.

The implication of the C-14 parameter values for biosphere dose conversion factors calculated in SwiBAC are presented in Section 7.2.

A side calculation, whereby the C-14 release to the biosphere is directed to the topsoil rather than the local aquifer is presented and discussed in Section 7.3.

7.1 Effective SwiBAC parameters

The effective soil solid/liquid partitioning coefficient (K_d) provided by Equation 63 is $0.015 \text{ m}^3 \text{ kg}^{-1}$ for the local aquifer, variably saturated zone and deep soil for all crops and biosphere-climate combinations.

Tab. 7-1 gives the effective K_d for the topsoil at equilibrium (Equation 65) and shows limited difference between crops (up to about 10%), whilst there is very little difference between the calculation cases. Tab. 7-1 shows that the C-14 model implies a greater degree of retention in the topsoil compared to the deep soil, variably saturated zone and local aquifer, reflecting a degree of additional retention of C-14 in organic matter. The table also provides an average value for the crops considered in SwiBAC (all crops except from the generic crop).

Tab. 7-1: Effective K_d for the topsoil.

K_d given in $[\text{m}^3 \text{ kg}^{-1}]$. The calculation cases are identified in Nagra (2024b).

Calculation case	Crop						
	Generic	Green vegetables	Root vegetables	Cereals	Fruit	Fodder	Average for modelled crops
Reference	2.7E-2	2.5E-2	2.6E-2	2.7E-2	2.6E-2	2.5E-2	2.6E-2
Warmer-drier	2.7E-2	2.5E-2	2.6E-2	2.7E-2	2.6E-2	2.5E-2	2.6E-2
Drained farmland	2.7E-2	2.5E-2	2.6E-2	-	-	2.5E-2	2.6E-2
Cold climate	2.6E-2	2.5E-2	2.5E-2	-	-	-	2.5E-2

Tab. 7-2 gives the effective soil-to-plant concentration ratios at equilibrium in the C-14 model (Equation 69). The results show that whilst there is a notable difference in the results for different crops (by up to a factor of about ten), there is very little difference in the values calculated between the calculation cases. This implies that, once C-14 has reached the soils, there is relatively little difference between the calculation cases in terms of the rate of uptake by plants from the soil (note that Section 6 identifies root uptake as being the key pathway for C-14 contamination of plants compared to uptake from the plant canopy atmosphere). The main contribution to variability in the results shown in Tab. 7-2 is the different degree of fractional water content in the crops; when that is accounted for, the differences between crops are relatively limited.

Tab. 7-2: Effective soil-to-plant concentration ratios
Ratios given for fresh weight plant and dry weight soil [-].

Calculation case	Crop					
	Generic	Green vegetables	Root vegetables	Cereals	Fruit	Fodder
Reference	2.7E+0	8.2E-1	1.8E+0	7.9E+0	8.4E-1	1.7E+0
Warmer-drier	2.7E+0	8.2E-1	1.8E+0	7.9E+0	8.4E-1	1.7E+0
Drained farmland	2.7E+0	8.2E-1	1.8E+0	-	-	1.7E+0
Cold climate	2.6E+0	8.1E-1	1.7E+0	-	-	-

Tab. 7-3 gives the additional loss rate from the topsoil calculated according to Equation 58. As with the effective K_d and the soil-to-plant concentration ratio, the results for the reference and warmer-drier cases are identical. However, the loss rate to atmosphere differs for the drained farmland and cold climate cases. For the drained farmland case, in which the groundwater table is closer to the soil surface, the average loss rate to atmosphere is marginally higher compared to the reference case. For the cold climate case, the average loss rate from the soil to the atmosphere is about 35% lower than the reference case. The differences between the calculation cases are smaller than the variability between the various crops.

Tab. 7-3: Effective additional loss rate from the topsoil
Loss rates given in [a^{-1}].

Calculation case	Crop						
	Generic	Green vegetables	Root vegetables	Cereals	Fruit	Fodder	Average for modelled crops
Reference	2.7E+0	3.1E-1	1.7E+0	2.1E+0	7.8E-1	5.5E-1	1.1E+0
Warmer-drier	2.7E+0	3.1E-1	1.7E+0	2.1E+0	7.8E-1	5.5E-1	1.1E+0
Drained farmland	3.7E+0	4.4E-1	2.3E+0	-	-	7.6E-1	1.2E+0
Cold climate	3.7E+0	2.3E-1	1.2E+0	-	-	-	7.1E-1

The effect of the model improvements on the parameter values calculated for SwiBAC is shown for the reference biosphere and a generic crop in Tab. 7-4 in comparison to Walke et al. (2013).

- The rate of loss of C-14 from the topsoil to the atmosphere is increased by about an order of magnitude, reflecting the change from a purely diffusive soil:atmosphere interface to one that recognises that turbulent mixing extends beyond the zero displacement plane within the plant canopy.
- The updated model results in a lower degree of C-14 accumulation in plant matter, with a factor of seven reduction in the soil-to-plant concentration ratio.
- This also means that less C-14 ends up in organic matter in the topsoil, thereby reducing the effective K_d by about a factor of eight.

Tab. 7-4: Comparison of C-14 parameters calculated for SwiBAC between the previous (Walke et al. 2013) and updated models for the reference case with a generic crop

Parameter	Previous value	Updated value
Additional loss rate from the topsoil	0.21 a ⁻¹	2.7 a ⁻¹
Soil-to-plant concentration ratio, expressed on a fresh weight plant:dry weight soil basis	19	2.7
K_d for the Topsoil	0.22 m ³ kg ⁻¹	0.027 m ³ kg ⁻¹

7.2 SwiBAC results

SwiBAC calculations have been undertaken with the updated parameter values for representing C-14 behaviour in the biosphere. SwiBAC 2.0 was used, with all other parameter values set to those adopted in Nagra 2024b.

- The source term to the local aquifer was set to 1 Bq kg⁻¹ for the reference biosphere case.
- The K_d in the local aquifer, variably saturated zone and deep soil were set to 0.015 m³ kg⁻¹ and that in the topsoil to 0.027 m³ kg⁻¹ (the value for the generic crop in Tab. 7-1).
- The degassing rate from the topsoil was set at 2.7 a⁻¹, consistent with that for a generic crop in Tab. 7-3.

The resulting amount calculated in the topsoil compartment of SwiBAC (green dotted line) is compared with the amount of C-14 in soil organic matter, topsoil solution and soil gas using the C-14 model (solid green line) in Fig. 7-1. The figure demonstrates that use of the effective K_d and the additional loss rate from the soil enables SwiBAC calculations to successfully reproduce the retention of C-14 within the topsoil that is observed in the C-14 model.

Fig. 7-1 also shows the retention of C-14 in the topsoil calculated by SwiBAC using a K_d for the topsoil of 0.026 m³ kg⁻¹ and a loss rate from the topsoil to elsewhere of 1.1 a⁻¹, which represent the average values for the crop types modelled in SwiBAC in Tab. 7-1 and Tab. 7-3. These values are appropriate for SwiBAC cases where no distinction is made in the modelling of different crop types (i.e. crops are grown/rotated over a single area of soil and a single consistent rate of irrigation is assumed across the modelled biosphere area). Fig. 7-1 shows that SwiBAC successfully reproduces a degree of retention for C-14 in the biosphere that sits between the lines for the individual crops when the crop-averaged rates are used.

SwiBAC includes the potential to model different soil areas with differing rates of irrigation. In this case, specific calculations would be required with the C-14 model to determine the most appropriate parameters to be used within the SwiBAC calculation.

The implications of the updated biosphere model for C-14 for the biosphere dose conversion factors (BDCFs) calculated with SwiBAC have been investigated by re-running SwiBAC calculations for both the reference and the warmer/drier climate conditions as documented in Nagra (2014) and Nagra (2024b).

The results are summarised in Tab. 7-3, which shows that accounting for an appropriate degree of atmospheric mixing within the plant canopy atmosphere reduces the calculated BDCFs for both reference and warmer/drier cases by about a factor of ten compared to Nagra (2014) (Tab. 7-5).

The contribution of different exposure pathways to the BDCF from Nagra (2014) and with the updated parameter values for C-14 is shown in Fig. 7-2. This shows that ingestion of animal produce and ingestion of crops contributed most to the BDCFs in Nagra (2014). The reduction in

calculated C-14 concentrations in crops and fodder resulting from the improvements to modelling of the plant canopy atmosphere means that, although they still contribute significantly, the contribution of ingestion of animal produce and crops to the BDCF is reduced, such that ingestion of groundwater now contributes up to about 25%.

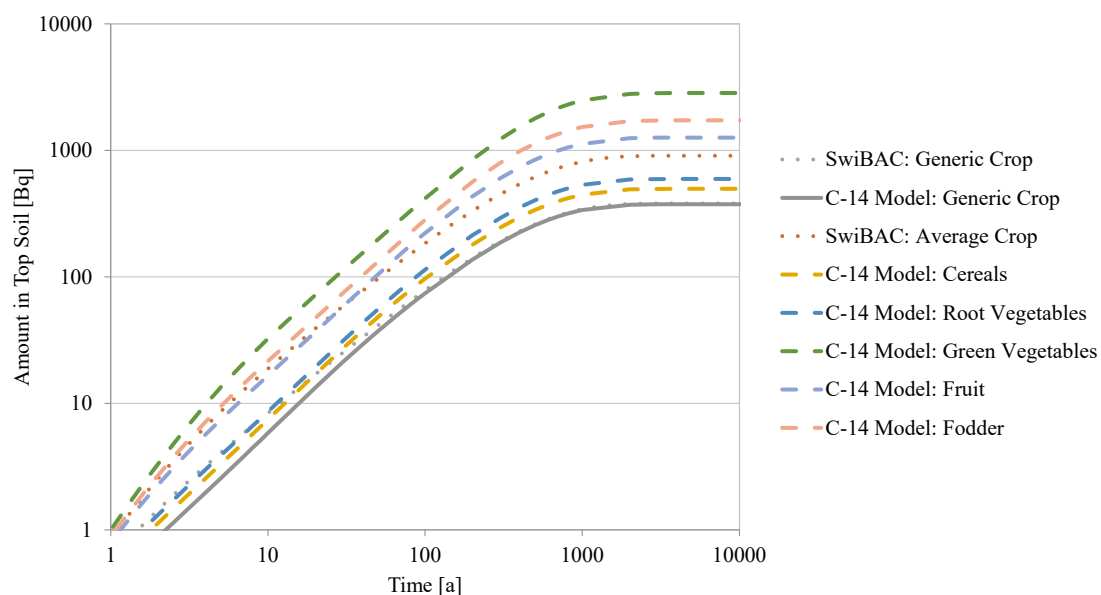


Fig. 7-1: Comparison of C-14 amounts in topsoil calculated with the C-14 model and SwiBAC for the reference biosphere
Amounts, $[Bq]$, are calculated with a unit source term of 1 Bq kg^{-1} to Local Aquifer.

Tab. 7-5: Biosphere dose conversion factors (BDCFs) calculated with SwiBAC
BDCF given in $[Sv \text{ Bq}^{-1}]$. BDCFs for drained farmland and cold climate conditions were not calculated in Nagra (2014), so there is no basis for comparison.

Calculation	Calculation case			
	Reference	Warmer/drier	Drained farmland	Cold climate
Nagra (2014)	3.7E-15	1.2E-14	-	-
Updated biosphere modelling for C-14	3.6E-16	9.2E-16	2.2E-16	1.0E-17

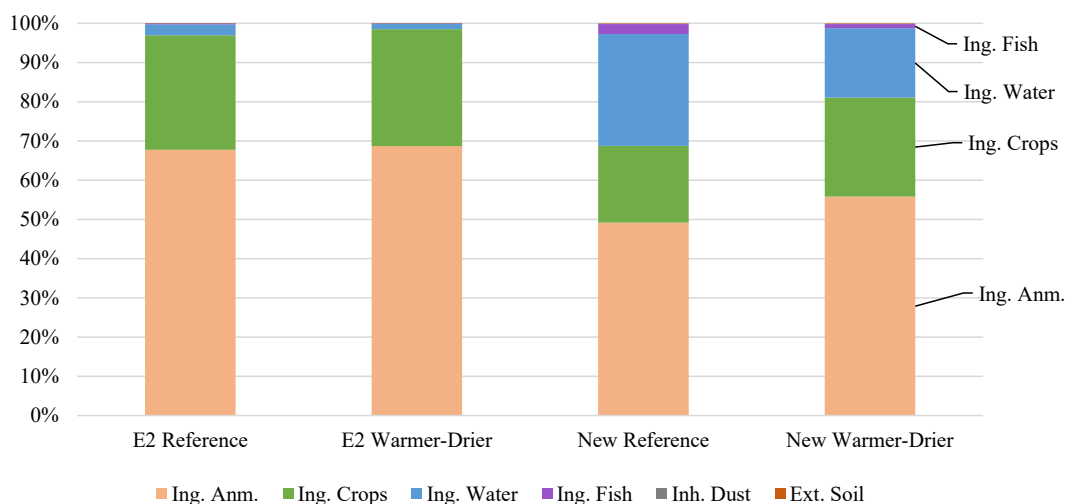


Fig. 7-2: Contribution of exposure pathways to the BDCF for C-14 from Nagra (2014) (for the Stage 2 of the Sectoral Plan E2) and with the updated modelling and parameter values for C-14 (for the general license application – RBG) for the reference and warmer-drier cases

The exposure pathways are: ingestion of animal produce (Ing. Anm.), ingestion of crops (Ing. Crops), ingestion of groundwater (Ing. Water), ingestion of fish from the river (Ing. Fish), inhalation of dust resuspended from the soil (Inh. Dust), and external irradiation from the soil (Ext. Soil).

It is noted in Section 2.1 that dissolved ^{14}C -methane and/or ^{14}C -carbon dioxide may form a gas phase in the shallow aquifer and/or in the deeper aquifer pathway, depending on its concentration and the local pressure, temperature and salinity conditions. The extent to which this might happen is uncertain. If this were to occur within the deeper aquifer pathway, then the gas phase may be trapped by low-permeability layers, and some C-14 will decay, while some will slowly redissolve into the groundwater. If this were to occur in the shallow aquifer (taken to be 20 m thick in reference calculations), then there is potential for the ^{14}C -methane or ^{14}C -carbon dioxide to migrate to surface soils via the gas pore-space in the unsaturated region above the water table.

A pessimistic side calculation has been undertaken to bound the potential dose consequences of this latter pathway, by undertaking a calculation with SwiBAC in which the unit C-14 source term to the biosphere (1 Bq a^{-1}) is directed to the topsoil rather than to the local aquifer. The calculation uses the same parameters for C-14 behaviour in the biosphere as above – i.e. there is an assumption that the release of methane and/or carbon dioxide is small relative to the overall carbon balance in the biosphere, such that amounts and fluxes of stable carbon are unaffected. This is pessimistic because it assumes 100% of the C-14 reaching the shallow aquifer in groundwater is immediately released to the gas phase and reaches the topsoil without delay or retardation. With reference assumptions, this calculation results in a BDCF for C-14 of $1.02\text{E-}15 \text{ Sv Bq}^{-1}$, which is a factor of 2.8 higher than when it is taken to remain in the aqueous phase.

Exposure rates to people for inhalation and ingestion of C-14 (Bq a^{-1}) are converted in SwiBAC to effective dose rates (Sv a^{-1}) using dose coefficients from the Swiss Radiological Protection Ordinance (RPO) (RPO 2021), which, in turn, are based on a compilation of the International Commission on Radiological Protection (ICRP 2012). In recent years, the ICRP have been reviewing and updating the basis for ingestion and inhalation dose coefficients (discussed in an

appendix to BIOPROTA (2023)). As a result of review and updated biokinetic modelling that supports the ICRP recommendations, it is expected that the dose coefficient for ingested C-14 may be about 30% of the current value used in SwiBAC (Harrison & Leggett 2016). Indeed, a value for C-14 ingested as bicarbonate (as may be appropriate to ingestion of inorganic carbon in drinking water) would be about 2.5% of the current value. Given that ingestion of C-14 in food and drinking water dominate potential exposures (see Fig. 7-2), then, when published by the ICRP, the updates will result in a further reduction in the BDCF.

8 Conclusions

An updated model for evaluating the dynamics of C-14 released from a deep geological repository to a local aquifer-soil-plant-atmosphere system is presented. The model draws on discussions and comparisons relating to C-14 modelling made within the international collaborative BIOPROTA programme, notably in improving the representation of dynamics within the plant canopy atmosphere, consistent with the latest research, standard micrometeorological models and other assessment programmes.

The model assumes that C-14 behaves in the same way as stable carbon and is based on masses and fluxes of stable carbon between various carbon pools. Organic matter represents the major carbon pool within the topsoil in comparison with the amount in exchangeable inorganic form. Relatively small amounts of carbon are present within the soil gas and the atmosphere around the plant, which are all subject to relatively high turnover rates (on a timescale of minutes for soil gas and a timescale of second for the plant canopy atmosphere). The degree of atmospheric exchange with the plant canopy atmosphere means that the small amount of plant carbon derived from root uptake of dissolved inorganic carbon dominates as a pathway for C-14 uptake by plants for a source-term to the soil.

Calculations with a unit source term of C-14 in groundwater to the local aquifer demonstrate a timescale of several hundred years to equilibrium, reflecting the relatively low turnover rate of carbon within the local aquifer itself.

As described in Walke et al. (2013), Nagra's previous model for C-14 in the biosphere adopted a pessimistic approach to representing mixing between the plant canopy atmosphere and the wider atmosphere. This aspect of the model has been improved, supported by recent research, by review within the BIOPROTA forum and by similar developments and refinements to models used for C-14 in the biosphere by other waste management organisations. By properly reflecting the degree of mixing between the plant canopy atmosphere and the wider atmosphere, the overall degree of plant uptake of C-14 released to the soil is reduced.

The C-14 model can be used to calculate effective parameter values needed to represent the behaviour of C-14 within Nagra's biosphere model SwiBAC. Calculations demonstrate that the difference between present-day and warmer-drier climate conditions has relatively very little effect on the calculated results. Potential dose consequence of releases to areas of land drained for farming and for releases during cold climate conditions are lower than the reference and warmer-drier climate assumptions, consistent with conclusions for other radionuclides in Nagra (2024b). The behaviour of C-14 in the more detailed C-14 model is shown to be successfully reproduced within SwiBAC by using the detailed model to calculate the following SwiBAC parameters:

- the effective solid/liquid distribution coefficients, K_d , values in the SwiBAC compartments;
- the loss term from the topsoil that reflects losses to the atmosphere and crops; and
- the effective soil-to-plant concentration ratios for the different crops considered.

A K_d value of $0.015 \text{ m}^3 \text{ kg}^{-1}$ is appropriate for the deep soil, variably saturated zone and the local aquifer for all crop types.

For the reference biosphere, the effective K_d for the topsoil is dependent on the crop being modelled, although the difference between crops is relatively limited (within about 10%). For the crops modelled in SwiBAC, the average effective K_d for the topsoil is $0.026 \text{ m}^3 \text{ kg}^{-1}$.

For the reference biosphere, the effective loss rate from the topsoil due to degassing varies by a factor of about ten between the different crop types, and has an average of about 1.1 a^{-1} .

For the reference biosphere, the effective soil-to-plant concentration ratios, expressed on a fresh weight plant and dry weight soil basis, vary from 0.82 for green vegetables to 7.9 for cereals for the cases studied. This variation is due largely to differences in the water content of the various crop types.

The overall impact of the updated C-14 model is to decrease the BDCF for C-14 by about a factor of ten for the reference (based on present-day climate) and warmer/drier conditions considered in Nagra (2014). The reduction in the degree of C-14 uptake by plants means that, while ingestion of food contaminated as a result of uptake by food and fodder crops still dominate in terms of potential exposure pathways, drinking of groundwater contributes about 25% of the calculated dose factor for the reference case.

There is potential for some fraction of C-14 in groundwater that discharges from depth to the near-surface to degas. If this were to happen in the local aquifer, then the associated C-14 may reach the overlying soil via the gas pore-space above the saturated zone. Calculations where 100% of the C-14 released to the biosphere is directed to the topsoil resulted in a BDCF that was a factor of 2.8 times higher than the reference case; this is taken to provide an upper bound for uncertainty about degassing in the near-surface. Further understanding of the gas source term and the pressure, temperature and salinity conditions from depth to the near-surface would help to better constrain this pathway in future.

Finally, it is noted that expected future updates to ICRP dose coefficients will reduce BDCFs for C-14 by at least 70%.

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