Biosphere Modelling for C-14: Description of the Nagra Model

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Nagra Working Reports concern work in progress that may have had limited review. They are intended to provide rapid dissemination of information.

This report was prepared by a project team consisting of Russell Walke (Quintessa Limited, UK), Fritz van Dorp (independent consultant, Switzerland) and Sven Keesmann (Nagra). The authors would like to thank Mike Thorne (Mike Thorne and Associates Limited) for a careful review of an earlier version of this report, which resulted in many valuable comments that were considered in preparing the final version. The project was managed by Sven Keesmann.
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. However, 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 model draws on discussions and comparisons relating to C-14 modelling made within the international BIOPROTA forum. The data for the model are described and justified, along with details of numerical implementation and illustrative calculations.

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 the flux of stable carbon through the upper part of the plant canopy and the atmospheric layer above the plants. Organic matter represents the major carbon pool within the top soil 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. Uptake of C-14 by plants from a layer within the canopy atmosphere that is conservatively represented as being diffusively-dominated is key in comparison to either root uptake from the top soil or uptake from a turbulent layer of the canopy atmosphere.

The 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 and the local aquifer
- additional loss term from the top soil to reflect losses to the atmosphere and crops
- 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 man and the environment. The Swiss radioactive waste management program 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). Nagra requires the capability to assess potential radiological exposures in the biosphere for comparison against regulatory protection criteria, should radionuclides be released from the barrier system of a deep geological repository and migrate to the surface environment over long periods of time after repository closure.

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 (Walke and Keesmann 2013) 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 for an element that is a fundamental building block of biological systems and for which such assumptions are more difficult to justify (Sheppard and Thorne 2005).

Intercomparison of models for C-14 in the biosphere forms the focus of a task within an international collaborative project, BIOPROTA (Norris et al. 2011). Such comparisons demonstrate the importance of representing the exchange of carbon between the soil, the canopy atmosphere and the turbulent atmosphere above the canopy. This has led to new models for C-14 that refine the representation of these features and processes (e.g. Limer et al. 2011, LLWR 2012).

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 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;
- the exchange of information between the C-14 model and Nagra's biosphere modelling code SwiBAC is discussed in Section 7;
- conclusions are drawn in Section 8.

References are provided at the end of the report.
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 relatively small at about 5%\(^1\) (NCRP 1984);
- the biosphere system is in steady state, such that stable carbon does not accumulate or deplete in the biosphere.

2.1 Basis

Radiocarbon may be released from radioactive waste repositories into the biosphere in the form of:

- gas as
  - CO\(_2\) or
  - methane
- carbon dissolved in water as
  - CO\(_2\) or bicarbonate
  - methane or
  - organic molecules

Methane will be oxidised to carbon dioxide in unsaturated soils and C-14 originally incorporated in the methane will become incorporated in the carbon dioxide.\(^2\) 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 and MacKenzie 2005). Organic molecules dissolved in water will also be oxidised to CO\(_2\) 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 the major part of their carbon from the atmosphere. Aquatic plants may derive a significant part from the water depending on the fraction of the plant which is submerged. However, local aquatic products are traditionally only of minor importance in the Swiss diet so they are not taken into account.

\(^1\) The isotopic fractionation varies between plant species and differs greatly between C\(_3\) (most food crops) and C\(_4\) (sugar cane, maize) pathways for photosynthesis. The maximum discrimination occurs in the C\(_3\) 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.
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 model\(^3\) (Coleman and Jenkinson 1999).

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 CO\(_2\) 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 the major part 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 CO\(_2\). From the soil gas phase, the CO\(_2\) can be released into the air layer above the soil due to diffusion or as a result 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 CO\(_2\) by the plant. This atmospheric carbon is partly derived from CO\(_2\) 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 effects of canopy structure on carbon dioxide transport and uptake by photosynthesis. The denser the canopy, the greater the degree of hold up of carbon dioxide released from the ground, but also the greater the degree of light attenuation in the upper part of the canopy reducing photosynthesis rates at the lower levels where soil-derived carbon dioxide concentrations are highest.

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.

Above-ground plant material or roots 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.

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\(^3\) The model ROTH-26.3, (Coleman and Jenkinson 1999) 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.
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. 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. 1 and the structure of the SwiBAC model (Walke and Keesmann 2013), 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 phase rather than the relatively small component that might become associated with solid inorganic material.

![Conceptual Model of Carbon Dynamics](image)

**Fig. 1:** Conceptual Model of Carbon Dynamics.

Notes: (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 top soil solution by the plant for use in photosynthesis within the plant leaves is assumed not to interact with the roots.

The source term considered is deep groundwater containing C-14 which discharges into a shallow local aquifer. Groundwater from the local aquifer is used for irrigation and it is taken that the C-14 in irrigation water is entirely transferred to the soil. Endpoints of the model calculations are C-14 concentrations and the C-14 specific activities (i.e. Bq kg\(_{C^{-1}}\)) in the different compartments.
Dissolved inorganic carbon in top soil solution, deep soil solution and the local aquifer is explicitly considered. Soil organic matter is explicitly considered in the top soil 4. Carbon in plant roots within the top soil is explicitly represented, as is carbon in the above-ground plants. Carbon in soil gas is explicitly represented 5. Carbon in the air above-ground is distinguished into a layer above the soil surface within which transport is taken to be dominated by diffusion and a layer above this within which turbulent mixing occurs and transport is dominated by advection. The height of the diffusive layer is approximately determined by the zero displacement height ($z_d$), which is within the plant canopy 6. The atmosphere outside the turbulent zone is represented as a sink for C-14.

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 river bed sediment compartments are represented as inert parts of the system with respect to carbon relevant processes.

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 top-soil solution with no interaction with the plant canopy 7. 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 Top Soil Solution to 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 top soil 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. 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. Diffusive gas exchange operates between the soil gas and the diffusive layer within the plant canopy and between the diffusive and turbulent layers. Diffusive exchange is also taken to operate from the top of the turbulent layer to the atmosphere above and horizontal advective transport which operates from the turbulent layer to the wider atmosphere removes radiocarbon out of the model.

Inorganic carbon is absorbed by the above-ground plant from the air within the canopy (which straddles both the diffusive and turbulent layers) and assimilated into organic plant material by photosynthesis. A reverse flux from the above-ground plant to the air within the canopy is

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4 Whilst it is possible to distinguish different forms of organic carbon within the soil (e.g. Coleman and 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 diffusive and the turbulent atmospheric layers. Although some organic matter occurs in soil at depth, most of it is concentrated in the top soil.

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

6 In reality, there will be advection and turbulent mixing also below $z_d$ (e.g. Foken 2008), however, its representation as a diffusion dominated layer is a conservative simplification because it will result in higher CO$_2$ concentrations and therefore higher C-14 concentrations.

7 Although foliar uptake is conceivable, outgassing will tend to release most of the C-14 and little will pass through the stomata.
caused by respiration. The long-term nature of C-14 releases to the biosphere via groundwater means that the diurnal cycle of photosynthesis and respiration is not explicitly represented; rather, average rates are adopted.

Exchange between the soil gas, the diffusive and turbulent atmosphere compartments is represented by diffusion. Instead of a photosynthesis model to predict the production of plant material, the annually produced plant material (a measured parameter) is used. 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 and minus respiration is added to the top soil organic matter. To keep a constant concentration of soil organic matter, the annual production of plant derived organic matter has to be decomposed at the same rate as it is added.
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
- fluxes of stable carbon between the compartments.

Transfer rates of C-14 within the biosphere system can then be calculated based on the transfer rates determined for stable carbon. The transfer rates then enable the behaviour of C-14 within the biosphere system to 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). 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 nomenclature adopted for the compartments considered is given in Table 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.

Tab. 1: Model Compartments of the C-14 Model.

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>Local Aquifer</td>
<td>LA</td>
</tr>
<tr>
<td>Surface Water</td>
<td>WS</td>
</tr>
<tr>
<td>Bed Sediment</td>
<td>WB</td>
</tr>
<tr>
<td>Deep Soil</td>
<td>DS</td>
</tr>
<tr>
<td>Top Soil</td>
<td>T</td>
</tr>
<tr>
<td>Top Soil Solution</td>
<td>TS</td>
</tr>
<tr>
<td>Top Soil Organic Matter</td>
<td>TO</td>
</tr>
<tr>
<td>Top Soil Gas</td>
<td>TG</td>
</tr>
<tr>
<td>Roots</td>
<td>PR</td>
</tr>
<tr>
<td>Above-ground Plant</td>
<td>PA</td>
</tr>
<tr>
<td>Diffusive Atmosphere</td>
<td>AD</td>
</tr>
<tr>
<td>Turbulent Atmosphere</td>
<td>AT</td>
</tr>
<tr>
<td>Wider Atmosphere</td>
<td>AW</td>
</tr>
<tr>
<td>Contaminated Source</td>
<td>SC</td>
</tr>
<tr>
<td>Uncontaminated Source</td>
<td>SU</td>
</tr>
<tr>
<td>Elsewhere</td>
<td>EW</td>
</tr>
</tbody>
</table>

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

\[
\frac{dN_i}{dt} = \left( \sum_{j \neq i} \lambda_{ji} N_j + \sigma_{MN} \lambda_N M_i + S_i \right) - \left( \sum_{j \neq i} \lambda_{ij} N_j + \lambda_N N_i \right)
\]  

[Bq \( a^{-1} \)] (1)

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),
- \( S_i \) [Bq \( a^{-1} \)] time-dependent external source of contaminant \( N \), i.e., C-14, to compartment \( i \),
- \( \lambda_M \) and \( \lambda_N \) [\( a^{-1} \)] decay constant for contaminants \( M \) and \( N \) respectively,
- \( \sigma_{MN} \) [-] branching ratio for decay from contaminant \( M \) to \( N \),
- \( \lambda_{ji} \) and \( \lambda_{ij} \) [\( a^{-1} \)] transfer coefficient representing the gain and loss of contaminant \( N \) from compartment \( i \) by transfer from and to compartment \( j \), respectively.\(^9\)

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 2011).

3.2 Stable Carbon Masses

The amount of exchangeable stable inorganic carbon in the Local Aquifer, Deep Soil and Top Soil solution is given by Equation 2. Note that for the Top Soil solution, the contributing parameters relate to the Top Soil as a whole:

\[
AC_i = f_{EC} \ f_{CC,i} \ f_{EC} \ C_{CC} \ V_i \ \rho_{b,i}
\]  

[kg C] (2)

- \( i \) compartment index \( LA, DS \) 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,

\(^9\) 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.
\( C_{fCC} \) \([\text{kgC/kgCaCO}_3]\) mass fraction of carbon in calcium carbonate,

\( V \) \([\text{m}^3]\) volume of the compartment,

\( \rho_b \) \([\text{kg m}^{-3}]\) dry bulk density of the compartment given by:

\[
\rho_{bi} = (1 - \theta_i) \rho_{gi} \quad [\text{kg m}^{-3}] \quad (3)
\]

\( \theta_i \) [-] total porosity of the compartment,

\( \rho_g \) \([\text{kg m}^{-3}]\) grain density of solid material in the compartment.

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

\[
AC_{TO} = f_{OM,T} C_{fOM} V_T \rho_{b,T} \quad [\text{kgC}] \quad (4)
\]

\( f_{OM,T} \) \([\text{kg kg}^{-1}]\) organic matter content of the top soil solid as a mass fraction,

\( C_{fOM} \) \([\text{kgC kg}^{-1}]\) mass fraction of carbon in organic matter,

\( V_T \) \([\text{m}^3]\) volume of Top Soil.

The amount of stable carbon in Surface Water and Bed Sediment is given by\(^\text{10}\):

\[
AC_i = C_{fw,i} \theta_w V_i \quad [\text{kgC}] \quad (5)
\]

\( i \) compartment index \( WS \) or \( WB \),

\( \theta_w \) [-] volumetric moisture content,

\( C_{fw} \) \([\text{kgC m}^{-3}]\) carbon content in the water.

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

\[
AC_i = A_f B_i C_{fOM} \quad [\text{kgC}] \quad (6)
\]

\( i \) compartment index \( PR \) or \( PA \),

\( A_f \) \([\text{m}^2]\) area of the agricultural land,

\( B \) \([\text{kg m}^{-2}]\) 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 turbulent and diffusive 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

\(^\text{10}\) 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.
most of the carbon within them originates from the overlying atmosphere. Therefore, the amount of stable carbon in both the Turbulent Atmosphere and Diffusive Atmosphere are given by:

$$AC_i = A_f \ h_i \ f_{CO2} \ C_{fCO2} \ \text{[kgC]} \ (7)$$

$i$ compartment index $AT$ or $AD$,
$h$ $[m]$ vertical thickness of the layer,
$f_{CO2}$ $[-]$ volumetric fraction of CO2 in the air above the canopy,
$C_{fCO2}$ $[\text{kgC} \ m_{CO2}^{-3}]$ is the mass of inorganic carbon in 1 m$^3$ of CO2.

As a result of the BIOPROTA studies relating to C-14 (e.g. Norris et al. 2011), there is on-going discussion regarding an appropriate height to assume for the height of the layer of the atmosphere above the soil surface that is dominated by diffusion (e.g. LLWR 2012). The diffusive layer will have higher concentrations of CO2 in comparison to the turbulent atmosphere and the wider atmosphere due to its release from the soil. In light of uncertainty about atmospheric mixing within the plant canopy, it is therefore conservative to assume that the thickness of the diffusive layer is maximised, such that the plant is exposed to C-14 at higher concentrations. Consistent with other models (e.g. Limer et al. 2011), the vertical thickness of the diffusive layer, $h_{AD}$, is taken to be the same as the zero displacement height, $z_d$, which can be estimated from the canopy height:

$$h_{AD} = z_d = R_{dc} \ z_C \ [m] \ (8)$$

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

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

$$h_{AT} = z_{10} - z_d = z_{10} - R_{dc} \ z_C \ [m] \ (9)$$

The concentration of stable carbon in Top Soil Gas is assumed to be higher than, but in equilibrium with, the Diffusive Layer, therefore the amount of carbon in the Top Soil Gas is given by:

$$AC_{TG} = E_f \ f_{CO2} \ C_{fCO2} \ (\theta_{t,T} - \theta_{w,T}) \ V_T \ [\text{kgC}] \ (10)$$

$E_f$ $[-]$ enhancement factor for the concentration of carbon in soil gas in comparison to the canopy atmosphere,
$\theta_{t,T}$ $[-]$ total porosity of the Top Soil,
$\theta_{w,T}$ $[-]$ water filled porosity (volumetric moisture content) of the Top Soil.

\[11\] The plant volume is considered negligible.
3.3 Stable Carbon Fluxes

Most stable carbon fluxes are explicitly parameterised and calculated, whereas others are determined by the flux required to balance the carbon contents in the donor compartment as defined in the previous section, given that the system is taken to be in steady state. The transfers that are explicitly calculated and those that are determined by the carbon balance are highlighted in Fig. 2.

Stable carbon fluxes, $F_C$, can occur from the uncontaminated and contaminated source to Local Aquifer and Surface Water, from Local Aquifer to Deep Soil, from Deep Soil to Local Aquifer, from Deep Soil to Top Soil Solution, from Top Soil Solution to Deep Soil, from Surface Water to Bed Sediment, from Bed Sediment to Surface Water, from Bed Sediment to Local Aquifer, from Bed Sediment to Local Aquifer, from Local Aquifer to Elsewhere and from Surface Water to Elsewhere:

$$F_{C_{i,j}} = F_{ij} C_{W_{j}} \text{ } [kgC \text{ } a^{-1}] \quad (11)$$

$F_{ij} \text{ } [m^3 \text{ } a^{-1}]$ water flux from compartments $i$ to $j$,  
$C_{W_{j}} \text{ } [kgC \text{ } m^{-3}]$ 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 source to the Local Aquifer.
The stable carbon fluxes due to irrigation from Local Aquifer to Top Soil Solution, $F_{LA\_TS}$, and from Surface Water to Top Soil Solution, $F_{WS\_TS}$, are given by:

$$FC_{LA\_TS} = F_{LA\_TS} CF_{w\_LA} (1 - f_{\text{degass}}) \quad [\text{kgC m}^{-3} \text{a}^{-1}] \quad (12)$$

$$FC_{WS\_TS} = F_{WS\_TS} CF_{w\_WS} (1 - f_{\text{degass}}) \quad [\text{kgC m}^{-3} \text{a}^{-1}] \quad (13)$$

- $F_{LA\_TS}$ [m$^3$ a$^{-1}$] irrigation water flux from the aquifer to the top soil,
- $F_{WS\_TS}$ [m$^3$ a$^{-1}$] irrigation water flux from the surface water to the top soil,
- $f_{\text{degass}}$ [-] 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 diffusive atmosphere. The stable carbon fluxes from Local Aquifer to the Diffusive Atmosphere, $F_{LA\_AD}$, and Surface Water to Diffusive Atmosphere$^{12}$, $F_{WS\_AD}$, are given by:

$$FC_{LA\_AD} = F_{LA\_TS} CF_{w\_LA} f_{\text{degass}} \quad [\text{kgC a}^{-1}] \quad (14)$$

$$FC_{WS\_AD} = F_{WS\_TS} CF_{w\_WS} f_{\text{degass}} \quad [\text{kgC a}^{-1}] \quad (15)$$

The stable carbon flux from the Wider Atmosphere to the Top Soil Solution, $FC_{AW\_TS}$, is given by:

$$FC_{AW\_TS} = d_{\text{precipit}} A_f C_{fp} \quad [\text{kgC a}^{-1}] \quad (16)$$

- $d_{\text{precipit}}$ [m a$^{-1}$] precipitation rate,
- $C_{fp}$ [kgC m$^{-3}$] carbon content in precipitation.

Transport vertically from the soil gas through the canopy to the atmosphere is treated as a diffusion-like process, where the diffusion coefficient $D$ is represented by:

$$D = \begin{cases} 
D_{\text{soil}} & \text{for } z \leq 0 \text{ m} \\
D_{\text{air}} & \text{for } 0 \text{ m} < z \leq z_d \\
D_{\text{air}} + k u^* (z - z_d) & \text{for } z > z_d 
\end{cases} \quad [\text{m}^2 \text{s}^{-1}] \quad (17)$$

- $k$ [-] von Kármán's constant,
- $u^*$ [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),
- $z$ [m] height in relation to the ground surface (determined by the compartment geometry),
- $D_{\text{soil}}$ [m$^2$ s$^{-1}$] effective diffusion coefficient for soil,
- $D_{\text{air}}$ [m$^2$ s$^{-1}$] molecular diffusion coefficient in free air.

$^{12}$ Note that there is no degassing from surface water direct to the wider atmosphere because the surface water is represented as a relatively inert part of the system with respect to carbon relevant processes, as described in Section 2.1.
The effective diffusion coefficient for soil, $D_{\text{soil}}$, is a fraction, $f_s$, of the free air value, $D_{\text{air}}$:

$$D_{\text{soil}} = f_s D_{\text{air}} \quad [\text{m}^2 \text{s}^{-1}]$$ (18)

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):

$$\Omega^{j,j+1} = \int_{\zeta^{h/j+1}}^{\zeta^{h/j}} \frac{dz}{D(z)} \quad [s \text{ m}^{-1}]$$ (19)

Where $\zeta$ represents the position of the interface, and $h$ is the vertical thickness of the layers.

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

$$\Omega^{j,j+1} = \frac{1}{2} \left( \frac{h^j}{D^j} + \frac{h^{j+1}}{D^{j+1}} \right) \quad [s \text{ m}^{-1}]$$ (20)

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

$$\lambda_{D}^{j,j+1} = \frac{1}{\Omega^{j,j+1}} \left( \frac{h^j}{D^j} \right) \quad [s^{-1}]$$ (21)

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

$$\lambda_{D}^{j+1,j} = \frac{1}{\Omega^{j+1,j}} \left( \frac{h^{j+1}}{D^{j+1}} \right) \quad [s^{-1}]$$ (22)

This provides the basis for calculating the diffusive exchange of stable carbon between the turbulent and diffusive atmosphere and the diffusive atmosphere and soil gas:

$$FC_{j,j+1} = \lambda_{D}^{j,j+1} AC_j \quad [\text{kg} \text{ C a}^{-1}]$$ (23)

$j$ index for compartment Top Soil Gas or Diffusive Atmosphere,

$j+1$ successor of $j$ in the sequence Turbulent Atmosphere, Diffusive Atmosphere, and Top Soil Gas.

The diffusive flux from the turbulent layer to the wider atmosphere needs not be explicitly calculated, as the loss from the compartment is determined by the carbon balance (see Fig. 2).

For completeness, a diffusive flux of stable carbon from the wider atmosphere to the Turbulent 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 turbulent 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 turbulent layer. The amount of stable carbon in the layer of the atmosphere involved in the

\[13\] Note that conversion between units of time from s\(^{-1}\) to a\(^{-1}\) is implicitly assumed.
diffusive exchange with the turbulent layer is therefore the same as the amount within the
turbulent layer, \( AC_{AW} = AC_{AT} \). Consistent with Equation 20, the transport resistance can be
declared as:

\[
\Omega^{AW,AT} = \frac{1}{2} \left( \frac{h^{AT}}{D^{AT}} + \frac{h^{AT}}{D^{AT}} \right) = \frac{h^{AT}}{D^{AT}} \quad [s \ m^{-1}] \quad (24)
\]

The total stable carbon flux from the wider atmosphere to Turbulent 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 Turbulent Atmosphere is
given by:

\[
FC_{AW,AT} = u_{AT} W_f h^{AT} f_{CO_2} C_fCO_2 + \lambda^{AW,AT}_{D} AC_{AW} \quad [kgC \ a^{-1}] \quad (25)
\]

\( u_{AT} \) \( [m \ a^{-1}] \) representative wind speed for the Turbulent Atmosphere,

\( W_f \) \( [m] \) width of the field,

\( h^{AT} \) \( [m] \) thickness of the turbulent layer,

\( \lambda^{AW,AT}_{D} \) \( [a^{-1}] \) transfer rate due to diffusion from the wider atmosphere (based on
Equations 22 and 24).

The wind speed at the mid-point of the turbulent 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
little impact on the wind speed at the mid-point of the turbulent layer, given the 10 m height of
the turbulent 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 \( z_d \) from\(^{14}\):

\[
u(z) = u_{10} \frac{\ln(z/z_d)}{\ln(z_{10}/z_d)} \quad [m \ s^{-1}] \quad (26)
\]

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 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.

\(^{14}\) Note that conversion between units of time from s\(^{-1}\) to a\(^{-1}\) is implicitly assumed.
Assuming a uniform wind rose, the width of the field, $W_f$, is taken as being:

$$W_f = 2\left(\frac{A_f}{\pi}\right)^\frac{1}{3} \quad [m] \quad (27)$$

The stable carbon flux from both Diffusive Atmosphere and Turbulent Atmosphere to Above Ground Plant, $F_{C_{\text{Air,PA}}}$, is given by:

$$F_{C_{\text{Air,PA}}} = F_{C_{\text{AD,PA}}} + F_{C_{\text{AT,PA}}}$$

$$= Y_{G,PA} A_f C f_{OM} (1 - f_{CS,PA}) + Y_{G,PR} A_f C f_{OM} (1 - f_{CS,PR}) \quad [kgC \, a^{-1}] \quad (28)$$

- $F_{C_{\text{AD,PA}}} [kgC \, a^{-1}]$ flux of stable carbon from Diffusive Atmosphere to Above Ground Plant,
- $F_{C_{\text{AT,PA}}} [kgC \, a^{-1}]$ flux of stable carbon from Turbulent Atmosphere to Above Ground Plant,
- $Y_{G,PA}, Y_{G,PR} [kg \, m^2 \, a^{-1}]$ gross dry weight annual assimilation of above-ground plants and roots,
- $f_{CS,PA}, f_{CS,PR} [-]$ fraction of carbon in Above Ground Plant or Root derived from the soil.
The gross annual assimilation, $Y_G$, is given by:

$$Y_{G,i} = \frac{Y_{N,i}}{1 - f_R} \quad [kg \ m^2 \ a^{-1}] \quad (29)$$

$i$ compartment index $PA$ or $PR$,

$Y_N \quad [kg \ m^2 \ a^{-1}]$ net dry weight production of organic matter per year,

$f_R \quad [-]$ respiration fraction of gross assimilation.

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:

$$Y_{N,i} = \frac{Y_{DW,i}}{f_H} \quad [kg \ m^2 \ a^{-1}] \quad (30)$$

$i$ compartment index $PA$ or $PR$,

$Y_{DW} \quad [kg \ m^2 \ a^{-1}]$ dry weight yield of harvested crop,

$f_H \quad [-]$ 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:

$$Y_{N,PR} = R_{RS} Y_{N,PA} \quad [kg \ m^2 \ a^{-1}] \quad (31)$$

$R_{RS} \quad [-]$ 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:

$$Y_{N,PA} = \frac{Y_{N,PR}}{R_{RS}} \quad [kg \ m^2 \ a^{-1}] \quad (32)$$

The dry weight yield of harvested crop is given by:

$$Y_{DW} = Y_{FW} (1 - f_w) \quad [kg \ m^2 \ a^{-1}] \quad (33)$$

$Y_{FW} \quad [kg \ m^2 \ a^{-1}]$ fresh weight yield of harvested material,

$f_w \quad [-]$ fractional water content of the harvested material.

Based on the model of Limer et al. (2011), the uptake from each atmosphere compartment can be determined on the basis of light intensity in the plant canopy. The fraction of plant carbon taken up from atmosphere that is drawn from the Diffusive Atmosphere, $f_{AD}$, is given by:

$$f_{AD} = \frac{\exp\left(\frac{R_K \cdot K \cdot LAI \cdot h_{AD}}{z_C}\right) - 1}{\exp(R_K \cdot K \cdot LAI) - 1} \quad [-] \quad (34)$$
$R_k$ [-] ratio of the extinction coefficient for carbon allocation to the extinction coefficient for diffuse light.

$K$ [-] extinction coefficient for diffuse light.

$LAI$ [-] leaf area index.

This function is illustrated in Fig. 4, assuming a canopy height of 1 m, a $LAI$ of 3.62, $K$ of 0.85 and $R_k$ of 0.4. The figure shows that proportionally more carbon is assimilated at the top of the plant canopy.

![Fraction of Carbon Assimilated from the Diffusive Layer](image)

**Fig. 4:** Fraction of Carbon Assimilated from the Diffusive Layer.

The flux of stable carbon from Diffusive Atmosphere to Above Ground Plant, $FC_{AD, PA}$, is given by:

$$FC_{AD, PA} = f_{AD} FC_{AIPL} \quad [kgC \text{ a}^{-1}] \quad (35)$$

Similarly, the flux of stable carbon from Turbulent Atmosphere to Above Ground Plant, $FC_{AT, PA}$, is given by:

$$FC_{AT, PA} = (1 - f_{AD}) FC_{AIPL} \quad [kgC \text{ a}^{-1}] \quad (36)$$
The stable carbon flux from Above Ground Plant to Diffusive Atmosphere and Turbulent Atmosphere due to plant respiration is taken to be distributed in the same way as photosynthetic assimilation. Therefore, the flux to Diffusive Atmosphere, \( FC_{PA,AD} \), is given by:

\[
FC_{PA,AD} = f_{AD} Y_{G,PA} f_{R,PA} A_f C_f OM
\]

[\text{kgC a}^{-1}] (37)

And the flux from the Above Ground Plant to the Turbulent Atmosphere, \( FC_{PA,AT} \), is given by:

\[
FC_{PA,AT} = (1 - f_{AD}) Y_{G,PA} f_{R,PA} A_f C_f OM
\]

[\text{kgC a}^{-1}] (38)

The stable carbon flux from Top Soil Solution to Above Ground Plant, \( FC_{TS,PA} \), is given by:

\[
FC_{TS,PA} = Y_{G,PA} A_f C_f OM f_{CS,PA} + Y_{G,PR} A_f C_f OM f_{CS,PR}
\]

[\text{kgC a}^{-1}] (39)

The stable carbon flux from Roots to Top Soil Solution, \( FC_{PR,TS} \), is given by:

\[
FC_{PR,TS} = A_f Y_{G,PR} f_{R,PR} C_f OM
\]

[\text{kgC a}^{-1}] (40)

The stable carbon flux from Above Ground Plant to Roots, \( FC_{PA,PR} \), is given by:

\[
FC_{PA,PR} = Y_{G,PR} A_f C_f OM
\]

[\text{kgC a}^{-1}] (41)

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:

\[
FC_{PA,EW} = A_f Y_{N,PA} f_{H,PA} C_f OM = A_f Y_{DW,PA} C_f OM
\]

[\text{kgC a}^{-1}] (42)

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:

\[
FC_{PR,EW} = A_f Y_{N,PR} f_{H,PR} C_f OM = A_f Y_{DW,PR} C_f OM
\]

[\text{kgC a}^{-1}] (43)

The stable carbon flux from Above Ground Plant to Top Soil Organic Matter, \( FC_{PA,TO} \), is given by:

\[
FC_{PA,TO} = Y_{N,PA} A_f C_f OM \left(1 - f_{H,PA}\right)
\]

[\text{kgC a}^{-1}] (44)

The stable carbon flux from Roots to Top Soil Organic Matter, \( FC_{PR,TO} \), is given by:

\[
FC_{PR,TO} = Y_{N,PR} A_f C_f OM \left(1 - f_{H,PR}\right)
\]

[\text{kgC a}^{-1}] (45)

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

\[
FC_{TO,TS} = FC_{PR,TO} + FC_{PA,TO}
\]

[\text{kgC a}^{-1}] (46)
The stable carbon flux from Top Soil Solution to Top Soil Gas, $F_{CTS,TG}$, is given by:\(^{15}\):

$$F_{CTS,TG} = F_{AW,TS} + F_{LA,TS} + F_{DS,TS} + F_{TO,TS} + F_{PR,TS} + F_{WS,TS} - F_{TS,DS} - F_{TS,PA} \quad [\text{kgC a}^{-1}] \quad (47)$$

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.

The stable carbon flux from Top Soil Gas to Diffusive Atmosphere, $F_{TG,AD}$, is given by:

$$F_{TG,AD} = F_{TS,AD} + F_{AD,TS} \quad [\text{kgC a}^{-1}] \quad (48)$$

The stable carbon flux from the Diffusive Atmosphere to the Turbulent Atmosphere, $F_{AD,AT}$, is given by:

$$F_{AD,AT} = F_{TG,AD} + F_{PA,AD} + F_{LA,AD} + F_{WS,AD} + F_{AT,AD} - F_{AD,TG} - F_{AD,PA} \quad [\text{kgC a}^{-1}] \quad (49)$$

The stable carbon flux from the Turbulent Atmosphere to the atmosphere elsewhere, $F_{AT,AW}$, is given by:

$$F_{AT,AW} = F_{AD,AT} + F_{AW,AT} + F_{PA,AT} - F_{AT,AD} - F_{AT,PA} \quad [\text{kgC a}^{-1}] \quad (50)$$

3.4 C-14 Transfer Model

A source flux, $SF$, equivalent to 1 Bq kgC\(^{-1}\) of C-14 in contaminated groundwater from the geosphere is introduced to the Local Aquifer according to:

$$SF = C_{GW} \cdot F_{SC,LA} \cdot C_{f,W,LA} \quad [\text{Bq a}^{-1}] \quad (51)$$

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

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

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

$$\lambda_{C-14,ij} = \frac{FC_{ij}}{AC_i} \quad [a^{-1}] \quad (52)$$

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

$FC_{ij}$ \quad [kgC a\(^{-1}\)] \quad flux of stable carbon,

$AC_i$ \quad [kgC] \quad amount of stable carbon in the donor compartment.

\(^{15}\) $F_{TS,TG}$ 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.
Specific activities, $SpA$, can be calculated for the modelled compartments according to:

$$SpA = \frac{N}{AC} \quad [\text{Bq kg}^{-1}C] \quad (53)$$

$N \quad [\text{Bq}]$ 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 which do not exist in the SwiBAC dynamic transport model. Moreover, the harvest of the crop and discharges to the wider atmosphere both result in a loss of C-14 from the system. Including in SwiBAC an additional loss term for C-14, which emanates from the top soil compartment, permits to take account of this net loss in the C-14 model. Furthermore, adjusting the effective distribution of C-14 between solid and liquid phases in the SwiBAC compartments Top Soil, Deep Soil 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 term, the effective distribution between solid and liquid phases and the soil-to-plant concentration ratios is 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 top soil 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 $TF_{i,j}$, then the net flux from the top soil, $TF_{\text{soil}}$, is given by:

$$TF_{\text{soil}} = TF_{T_{G},AD} + TF_{T_{S},P_{4}} - TF_{A_{D},T_{G}} - TF_{P_{R},T_{S}} - TF_{P_{R},T_{O}} - TF_{P_{A},T_{O}} \quad [\text{Bq a}^{-1}] \quad (54)$$

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

This can be converted into a net loss rate, $\lambda_{\text{soil}}$, by comparison with the amount of C-14 in the top soil:

$$\lambda_{\text{soil}} = \frac{TF_{\text{soil}}}{N_{T_{S}} + N_{T_{O}} + N_{T_{G}}} \quad [\text{a}^{-1}] \quad (55)$$

$N_i \quad [\text{Bq}]$ calculated amount of C-14 in compartment $i$ at steady state.
3.5.2 Effective Distribution between Solid and Liquid Phases

In both SwiBAC and the C-14 model, transfers between the top soil, deep soil 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):

\[
\lambda_{ij} = \frac{F_{ij}}{(\theta_{ij} + \rho_{b,i} K_{d,ij}) V_i} \quad [a^{-1}] \quad (56)
\]

Within the C-14 model, the rates for these transfers are based on Equations 2, 11 and 52, such that the transfer rate is given by:

\[
\lambda_{ij} = \frac{F_{ij} C_{f_{W,i}}}{f_{EC} f_{CC,i} C_{f_{CC}} V_i \rho_{b,i}} \quad [a^{-1}] \quad (57)
\]

The rates for these transfers in the C-14 model can be replicated in SwiBAC by calculating effective \( K_d \) values by rearranging Equation 56:

\[
K_{d,i} = \frac{F_{ij} - \theta_{ij} \lambda_{ij} V_i}{\lambda_{ij} \rho_{b,i} V_i} \quad [m^3 kg^{-1}] \quad (58)
\]

Substituting Equation 57 into Equation 58, the flow rates and volumes cancel out, such that the effective \( K_d \) values can be calculated using:

\[
K_{d,i} = \frac{f_{EC} f_{CC,i} C_{f_{CC}}}{C_{f_{W,i}}} \theta_{W,i} \quad [m^3 kg^{-1}] \quad (59)
\]

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

\[
K_{d,i} = \frac{f_{EC} f_{CC,i} C_{f_{CC}}}{C_{f_{W,i}}} \quad [m^3 kg^{-1}] \quad (60)
\]

\( i \) compartment index DS or LA.

This expression provides a means of calculating the \( K_d \) value for the deep soil and aquifer compartments in SwiBAC, which are each represented with a single compartment in both models. However, for the SwiBAC top soil 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 top soil to the deep soil conceptually invariant for both models the transfer rate \( \lambda_{TS,DS} \) relating to Top Soil Solution has to be re-scaled to \( \lambda_{T,D} \) relating to the total Top Soil.

\[
\lambda_{T,D} = \frac{N_{TS}}{N_{TS} + N_{TO} + N_{TG}} \lambda_{TS,DS} \quad [a^{-1}] \quad (61)
\]

\( N_i \) [Bq] calculated amount of C-14 in compartment \( i \) at steady state.
The distribution coefficient between the solid and liquid phase for Top Soil effectively becomes:

\[
K_{d,T} = \frac{N_{TS} + N_{TO} + N_{TG} \cdot f_{EC} \cdot f_{CC,TS} \cdot C_{f,CC}}{N_{TS} \cdot C_{f,w,TS}} \quad [m^3 \text{ kg}^{-1}]
\] (62)

### 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:

\[
C_{PA} = \frac{N_{PA} \cdot (1-f_{w})}{A_{f} \cdot B_{PA}} \quad [\text{Bq kg}_{\text{fresh}}^{-1}]
\] (63)

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

\[
C_{PR} = \frac{N_{PR} \cdot (1-f_{w})}{A_{f} \cdot B_{PR}} \quad [\text{Bq kg}_{\text{fresh}}^{-1}]
\] (64)

The activity concentration in top soil per dry weight, \(C_{T}\), is given by:

\[
C_{T} = \frac{N_{TS} + N_{TO} + N_{TG}}{V_{T} \cdot \rho_{h,T}} \quad [\text{Bq kg}_{\text{dry}}^{-1}]
\] (65)

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.

\[
CR = \frac{C_{PA}}{C_{T}} \quad \text{or} \quad CR = \frac{C_{PR}}{C_{T}} \quad [\text{Bq kg}_{\text{fresh}}^{-1} \quad \text{or} \quad \text{Bq kg}_{\text{dry}}^{-1}]
\] (66)

### 3.5.4 Interfacing the Dynamic Transport Model and the Exposure Model

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

Originally, the only possible losses of radionuclides from the system are the out-fluxes of radio- nuclides 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 term) in order to make the distribution of C-14 in SwiBAC match the distribution of the radionuclide in the C-14 model. Conceptually, these fluxes result in an exposure of humans by ingestion or inhalation, though the additional loss term is not directly taken into account by the exposure model in SwiBAC. Instead, ingestion via harvest is considered 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 rate. These pathways are parameterised in such a way that the corresponding fluxes match the fluxes calculated from the C-14 model.

\footnote{Details are to be found in (Walke and Keesmann 2013).}
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. 2 and the values are based on those as given in Nagra (2010). 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. 2: System-dependent Parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V$</td>
<td>$[m^3]$</td>
</tr>
<tr>
<td>$\theta_t$</td>
<td>[-]</td>
</tr>
<tr>
<td>$\theta_w$</td>
<td>[-]</td>
</tr>
<tr>
<td>$\rho_g$</td>
<td>$[kg \ m^{-3}]$</td>
</tr>
<tr>
<td>$A_f$</td>
<td>$[m^2]$</td>
</tr>
<tr>
<td>$F$</td>
<td>$[m^3a^{-1}]$</td>
</tr>
<tr>
<td>$d_{\text{precipit}}$</td>
<td>$[ma^{-1}]$</td>
</tr>
</tbody>
</table>

4.2 Crop-independent Parameters

The required crop-independent parameters are given in Tab. 3. 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 ($C_{n}H_{2n}O_{n}$ assumed).

B. The inorganic carbon content in water depends on many factors (see e.g. Kirby and Cravotta 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.

C. The concentration of CO$_2$ in the soil atmosphere is expected to be enriched by a factor of between 30 to 60 in comparison to the above-ground atmosphere. A reference value of 30 is adopted, consistent with Limer et al. (2011).
Tab. 3: Crop-Independent Parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{f_{CC}}$ [-]</td>
<td>Mass fraction of carbon in calcium carbonate</td>
<td>0.12</td>
<td>Based on CaCO$_3$</td>
</tr>
<tr>
<td>$C_{f_{CO2}}$ [kg cm$^{-3}$]</td>
<td>Mass of inorganic carbon in 1 m$^3$ of CO$_2$</td>
<td>$12 \frac{g_C}{22.4 L}$</td>
<td>1 mol CO$_2$ occupying 22.4 L at standard temperature and pressure.</td>
</tr>
<tr>
<td>$C_{f_{OM}}$ [-]</td>
<td>Mass fraction of carbon in organic matter</td>
<td>0.4</td>
<td>A</td>
</tr>
<tr>
<td>$C_{f_P}$ [kg cm$^{-3}$]</td>
<td>Carbon content in precipitation</td>
<td>0.04</td>
<td>Taken to be the same as $C_{f_W}$</td>
</tr>
<tr>
<td>$C_{f_W}$ [kg cm$^{-3}$]</td>
<td>Carbon content in the appropriate water</td>
<td>0.04</td>
<td>B</td>
</tr>
<tr>
<td>$E_f$ [-]</td>
<td>Enhancement factor for the concentration of stable carbon in the soil gas in comparison to the canopy atmosphere</td>
<td>30</td>
<td>C</td>
</tr>
<tr>
<td>$f_{CC}$ [-]</td>
<td>Mass fraction of the compartment solid as calcium carbonate</td>
<td>0.05</td>
<td>D</td>
</tr>
<tr>
<td>$f_{CO2}$ [-]</td>
<td>Volumetric fraction of CO$_2$ in the air above the canopy</td>
<td>0.0004</td>
<td>E</td>
</tr>
<tr>
<td>$f_{CS}$ [-]</td>
<td>Fraction of root or above-ground plant carbon derived from the soil</td>
<td>0.02</td>
<td>F</td>
</tr>
<tr>
<td>$f_{degass}$ [-]</td>
<td>Fraction of carbon content in irrigation water lost to the atmosphere due to degassing</td>
<td>0</td>
<td>Conservative modelling assumption</td>
</tr>
<tr>
<td>$f_{EC}$ [-]</td>
<td>Exchangeable carbonate as a mass fraction of the total carbonate</td>
<td>0.1</td>
<td>D</td>
</tr>
<tr>
<td>$f_{OM}$ [-]</td>
<td>Organic matter content of the top soil solid as a mass fraction</td>
<td>0.05</td>
<td>G</td>
</tr>
<tr>
<td>$f_R$ [-]</td>
<td>Respiration fraction of gross organic matter assimilation by plants</td>
<td>1/3</td>
<td>H</td>
</tr>
<tr>
<td>$k$ [-]</td>
<td>von Kármán's constant</td>
<td>0.41</td>
<td>Zhang et al. (2008)</td>
</tr>
<tr>
<td>$u^*$ [m s$^{-1}$]</td>
<td>Friction velocity</td>
<td>0.2</td>
<td>Reasonable value for crops</td>
</tr>
<tr>
<td>$R_{dc}$ [-]</td>
<td>Ratio of the zero displacement height to that of the top of the canopy of the dominant plant species</td>
<td>2/3</td>
<td>I</td>
</tr>
<tr>
<td>$D_{air}$ [m$^2$ s$^{-1}$]</td>
<td>Molecular diffusion coefficient in free air</td>
<td>1.4E-5</td>
<td>Lide (2006)</td>
</tr>
<tr>
<td>$f_s$ [-]</td>
<td>Ratio of the diffusion coefficient in soil to that in free air</td>
<td>0.1</td>
<td>J</td>
</tr>
<tr>
<td>$u_o$ [m s$^{-1}$]</td>
<td>Wind speed at 10 m height above ground</td>
<td>5</td>
<td>K</td>
</tr>
</tbody>
</table>
D. The model includes compartments for soil organic matter and CO₂ / 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 \( K_d \). For this purpose, the \( K_d \) value for C-14 of 5 L kg\(^{-1}\) in Nagra (2003) is 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 2000 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 CO₂ is taken to be 400 ppmv, which is slightly higher than present day value (385 ppmv), but 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 and 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 and 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.

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 and 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. 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 and Pröhl (2008) report heights for farmlands and forests, which are $\frac{1}{4}$ and $\frac{1}{5}$ of the vegetation height, respectively. A reference value of two-thirds is adopted here, consistent with Allen et al. (1998).

J. 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 $1.4 \times 10^{-5}$ m$^2$ s$^{-1}$. In forest soils, values of $f_s$ of 0.03 to 0.15 have been measured, and a reference value of 0.1 is used here, consistent with Limer et al. (2008).

K. 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 (Walke and Keesmann 2013). 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, 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 values for the leaf area index are based on data in Scurlock et al. (2001). Cropland values are assumed for the plants consumed directly by humans, and a grassland value is assumed for pasture.

D. The assumptions for the extinction coefficient are based upon the ranges observed for broadleaf species and grasses by Monsi and Saeki (1953). The mid-point of each range is the recommended value.

E. The assumption is based on observed ratios of the extinction coefficient for nitrogen allocation to that of diffuse light in Anten (1997). The value is potentially crop-dependent, although a single value is used here, which is consistent with Limer et al. (2011).

F. The fresh weight crop yields are based on Nagra (2003).

G. Assumption of net dry weight organic matter production rates of 2 kg m$^{-2}$ a$^{-1}$ for both the above-ground plant and roots is adopted for the generic crop.
Tab. 4: Crop-Dependent Parameters.
Notes on the adopted values are given in the text.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description and Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Generic Crop</td>
<td>Cereals</td>
<td>Root Vegetables</td>
</tr>
<tr>
<td>$f_{H}$</td>
<td>Fraction of the plant that is harvested</td>
<td>Above-ground</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>Below-ground</td>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>$f_w$</td>
<td>Fractional water content of the harvested material, [-]</td>
<td>-</td>
<td>0.1</td>
</tr>
<tr>
<td>$H_{AC}$</td>
<td>Height of the plant canopy, [m]</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$K$</td>
<td>Extinction coefficient for light, [-]</td>
<td>0.85</td>
<td>0.85</td>
</tr>
<tr>
<td>$R_K$</td>
<td>Ratio of the extinction coefficient for carbon allocation to the extinction coefficient for diffuse light, [-]</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>$R_{RS}$</td>
<td>Dry weight root:shoot ratio, [-]</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$Y_{FW}$</td>
<td>Fresh weight yield of harvested material, [kg m(^{-2}) a(^{-1})]</td>
<td>-</td>
<td>0.607</td>
</tr>
<tr>
<td>$Y_N$</td>
<td>Net dry weight production of organic material, [kg m(^{-2}) a(^{-1})]</td>
<td>Above-ground</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Below-ground</td>
<td>2</td>
<td>-</td>
</tr>
</tbody>
</table>
## Implementation

The model has been implemented in the AMBER generic compartment modelling software (Quintessa 2011). A screenshot is shown in Fig. 5. Data for a Temperate climate and a Warm/Dry climate given in Nagra (2010) 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:** 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.
6 Illustrative Calculations

An interaction matrix showing the stable carbon masses and balance for the Temperate climate with a generic crop is shown in Tab. 5. The table shows the relatively small amount of carbon within the soil gas, the diffusive atmosphere and the turbulent atmosphere compartments. The table also shows the dominance of the stable carbon flux through the turbulent atmosphere.

The amount of C-14 in the model compartments for a unit source term of 1 Bq kg_c^{-1} to the local aquifer is shown in Fig. 6 for the generic crop. The figure shows that it takes the system about 1000 years to reach an equilibrium, which is determined by the relatively slow turnover rate of stable carbon in the local aquifer (Tab. 5 implies a characteristic time of retention within the local aquifer of about 450 years). Retention within the 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. Turnover rates in other modelled compartments are relatively rapid (faster than once per year). Tab. 6 summarizes amounts and fluxes of C-14 in the model for a generic crop at equilibrium.

For a generic crop, the fraction of the plant carbon that is drawn from the diffusive atmosphere compartment is about 52 % (Equation 34), with the remaining fraction being drawn from the atmosphere around the top of the plant canopy where the light intensity is greatest. However, the concentration of C-14 within the diffusive atmosphere is higher (1E-7 Bq m^{-3} at equilibrium for a unit source flux to the local aquifer) than that within the turbulent atmosphere (1E-10 Bq m^{-3}). As a result, the plant draws about 1000 times as much of its C-14 contamination from the diffusive atmosphere in comparison to the turbulent layer.

Fig. 7 shows the resulting plant concentrations and associated specific activity for the generic crop, whilst Fig. 8 shows the effective soil-to-plant concentration ratios for different crops (Equation 66). The concentration ratios show an initial peak within the first five years before equilibrium is reached between five hundred and one thousand years.

The additional loss rate from the top soil (Equation 55) is shown in Fig. 9 for the generic crop.
Tab. 5: Interaction Matrix of Stable Carbon for the Temperate Climate with a Generic Crop.

Stable carbon masses, [kgC], are given in the leading diagonal elements, stable carbon fluxes, [kgC a⁻¹], are given in the off-diagonal elements (interactions are illustrated in a clock-wise direction).

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Local Aquifer</td>
<td>5.788E+07</td>
<td>0.000E+00</td>
<td>1.008E+05</td>
<td>2.730E+04</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Deep Soil</td>
<td>6.370E+04</td>
<td>4.341E+06</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>4.681E+08</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Surface Water</td>
<td></td>
<td>4.550E+04</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Bed Sediments</td>
<td>0.000E+00</td>
<td>1.008E+05</td>
<td>7.000E+02</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Top Soil Solution</td>
<td>6.370E+04</td>
<td>5.426E+05</td>
<td>2.675E+06</td>
<td>1.092E+05</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Top Soil Gas</td>
<td></td>
<td>3.656E+02</td>
<td>2.811E+06</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Diffusive Atmosphere</td>
<td>1.360E+05</td>
<td>3.250E+02</td>
<td>9.914E+05</td>
<td>2.807E+06</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Turbulent Atmosphere</td>
<td>6.458E+05</td>
<td>4.550E+03</td>
<td>2.544E+06</td>
<td>1.041E+09</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Above-Ground Plant</td>
<td>4.774E+05</td>
<td>4.326E+05</td>
<td>1.820E+06</td>
<td>2.730E+06</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
</tr>
<tr>
<td>Below-Ground Plant</td>
<td>9.100E+05</td>
<td>4.326E+05</td>
<td>1.820E+06</td>
<td>2.730E+06</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
<td>9.100E+05</td>
</tr>
<tr>
<td>Top Soil Organic Matter</td>
<td>1.820E+06</td>
<td>1.809E+07</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
<tr>
<td>Elsewhere</td>
<td>6.440E+04</td>
<td>4.680E+08</td>
<td>9.100E+04</td>
<td>1.043E+09</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
<td>0.000E+00</td>
</tr>
</tbody>
</table>
Tab. 6: Amounts and Fluxes of C-14 (for Equilibrium Conditions) for the Temperate Climate with a Generic Crop.
C-14 activities, \([Bq]\), are given in the leading diagonal elements, C-14 fluxes, \([Bq \text{ a}^{-1}]\), are given in the off-diagonal elements (interactions are illustrated in a clockwise direction).

<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Local Aquifer</td>
<td>2.244E+06</td>
<td></td>
<td></td>
<td>3.909E+03</td>
<td>1.059E+03</td>
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<tr>
<td>Deep Soil</td>
<td>3.860E+01</td>
<td>2.630E+03</td>
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<td>Surface Water</td>
<td></td>
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<td>3.799E-01</td>
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<td>3.909E+03</td>
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<td>3.909E+03</td>
<td>2.714E+01</td>
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<td>Top Soil Solution</td>
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<td>5.426E+05</td>
<td>1.635E+03</td>
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<td>Top Soil Gas</td>
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<td></td>
<td>2.207E-01</td>
<td>1.697E+03</td>
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<td></td>
<td>1.501E-01</td>
<td>4.578E+02</td>
<td>1.296E+03</td>
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<tr>
<td>Turbulent Atmosphere</td>
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<td></td>
<td>3.499E-01</td>
<td>2.465E-03</td>
<td>1.378E+00</td>
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<tr>
<td>Above-Ground Plant</td>
<td>1.193E+02</td>
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<td>1.081E+02</td>
<td>4.548E+02</td>
<td>6.822E+02</td>
<td>2.274E+02</td>
<td>2.274E+02</td>
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<tr>
<td>Below-Ground Plant</td>
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<td></td>
<td></td>
<td></td>
<td>4.548E+02</td>
<td>2.274E+02</td>
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<td></td>
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<td>Top Soil Organic Matter</td>
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<tr>
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<td>0.000E+00</td>
<td>0.000E+00</td>
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<td></td>
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</tr>
</tbody>
</table>
Fig. 6: Amount of C-14 in Compartments for the Temperate Climate. Amounts [Bq] are calculated for the generic crop.

Fig. 7: Above-Ground Plant Concentration and Specific Activity. Quantities are calculated for the generic crop and the Temperate climate.
Fig. 8: Effective Soil-to-Plant Concentration Ratios for the Temperate Climate.

Fig. 9: Loss Rate from the Top Soil for the Temperate Climate with a Generic Crop.
7 Integration within SwiBAC

The relationship between the C-14 model and the SwiBAC model is discussed in Section 3.5. This section presents the parameter values that are needed to replicate the behaviour of C-14 within the SwiBAC model using the models and data described above.

7.1 Effective SwiBAC Parameters

The effective soil solid/liquid partitioning coefficient (\(K_d\)) provided by Equation 60 is 0.015 m³ kg⁻¹ for the local aquifer and deep soil for all crops and biosphere-climate combinations. Tab. 7 gives the effective \(K_d\) for the top soil at equilibrium (Equation 62) and shows up to a factor of about three difference between crops, whilst there is no difference between climate states. For comparison, a \(K_d\) of 0.015 m³ kg⁻¹ was used in the calculations that supported the BDCF's presented in Nagra (2010); Tab. 7 shows that the C-14 model implies a greater degree of retention in the top soil.

Tab. 7: Effective \(K_d\) for the Top Soil.

\(K_d\) given in [m³ kg⁻¹]:

<table>
<thead>
<tr>
<th>Climate</th>
<th>Crop</th>
<th>Generic</th>
<th>Green Vegetables</th>
<th>Root Vegetables</th>
<th>Cereals</th>
<th>Fruit</th>
<th>Fodder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperate</td>
<td></td>
<td>2.19E-1</td>
<td>6.87E-2</td>
<td>1.64E-1</td>
<td>2.10E-1</td>
<td>1.14E-1</td>
<td>1.10E-1</td>
</tr>
<tr>
<td>Warm/Dry</td>
<td></td>
<td>2.19E-1</td>
<td>6.87E-2</td>
<td>1.64E-1</td>
<td>2.10E-1</td>
<td>1.14E-1</td>
<td>1.10E-1</td>
</tr>
</tbody>
</table>

Tab. 8 gives the effective soil-to-plant concentration ratios at equilibrium in the C-14 model (Equation 66). The results show that whilst there is a notable difference in the results for different crops (by up to a factor of about twelve), there is no difference in the values calculated for the two different climate states. For comparison, soil-to-plant concentration ratios of 0.3 were used for green vegetables, root vegetables, fruit and fodder and a value of 2 was used for grain in the calculations that supported the BDCF's presented in Nagra (2010). The values given in Tab. 8 therefore imply a greater degree of uptake from the soil.

Tab. 8: Effective Soil-to-Plant Concentration Ratios.

Ratios given for fresh weight plant and dry weight soil [-].

<table>
<thead>
<tr>
<th>Climate</th>
<th>Crop</th>
<th>Generic</th>
<th>Green Vegetables</th>
<th>Root Vegetables</th>
<th>Cereals</th>
<th>Fruit</th>
<th>Fodder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperate</td>
<td></td>
<td>1.87E+1</td>
<td>1.58E+0</td>
<td>3.64E+0</td>
<td>1.67E+1</td>
<td>1.74E+0</td>
<td>3.48E+0</td>
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<tr>
<td>Warm/Dry</td>
<td></td>
<td>1.87E+1</td>
<td>1.58E+0</td>
<td>3.64E+0</td>
<td>1.67E+1</td>
<td>1.74E+0</td>
<td>3.48E+0</td>
</tr>
</tbody>
</table>

Tab. 9 gives the additional loss rate from the top soil calculated according to Equation 55. Similar to the soil-to-plant concentration ratios and the \(K_d\) values, there is no difference between the different climate states considered. However, the various crops produce up to about a two-fold difference.
Tab. 9: Effective Additional Loss Rate from the Top Soil.
Loss rates given in \([a^{-1}]\).

<table>
<thead>
<tr>
<th>Climate</th>
<th>Crop</th>
<th>Generic</th>
<th>Green Vegetables</th>
<th>Root Vegetables</th>
<th>Cereals</th>
<th>Fruit</th>
<th>Fodder</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperate</td>
<td></td>
<td>2.10E-1</td>
<td>1.06E-1</td>
<td>2.02E-1</td>
<td>1.66E-1</td>
<td>1.46E-1</td>
<td>1.07E-1</td>
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<tr>
<td>Warm/Dry</td>
<td></td>
<td>2.10E-1</td>
<td>1.06E-1</td>
<td>2.02E-1</td>
<td>1.66E-1</td>
<td>1.46E-1</td>
<td>1.07E-1</td>
</tr>
</tbody>
</table>

Overall, the \(K_d\) and soil-to-plant concentration ratios given above will tend to increase retention and plant uptake of C-14 in comparison to previous calculations with SwiBAC. However, the inclusion of the additional loss term from the top soil to represent processes specifically appropriate to C-14 will tend to reduce retention in the top soil.

7.2 SwiBAC Results

SwiBAC calculations have been undertaken, in which the source term to the local aquifer is set at 1 Bq kgC\(^{-1}\) for the case with the Temperate climate.\(^7\) The \(K_d\) in the local aquifer and deep soil were set to 0.015 m\(^3\) kg\(^{-1}\) and that in the top soil to 0.219 m\(^3\) kg\(^{-1}\). (value for generic crop in Tab. 7) An additional transfer from the Top Soil to Elsewhere was included with a rate of 0.210 a\(^{-1}\), consistent with that for a generic crop in Tab. 9. The resulting amount calculated in the top soil compartment of SwiBAC (green dotted line) is compared with the amount of C-14 in soil organic matter, top soil solution and soil gas using the C-14 model (solid green line) in Fig. 10. 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 top soil that is observed in the C-14 model.

Fig. 10 also shows the retention of C-14 in the top soil calculated by SwiBAC using a \(K_d\) for the top soil of 0.133 m\(^3\) kg\(^{-1}\) and a loss rate from the top soil to elsewhere of 0.145 a\(^{-1}\), which represent the average values for the crop types modelled in SwiBAC. This rate is appropriate for SwiBAC cases where no distinction is made in the modelling of different crop types (i.e. a single consistent rate of irrigation is assumed across the modelled biosphere area).

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 new C-14 model for the biosphere dose conversion factors (BDCFs) calculated with SwiBAC have been investigated by running the following calculations for both the Temperate and the Warm/Dry climate conditions as documented in Nagra (2010):

- Calculation of BDCFs with the original settings using SwiBAC;
- Calculation using the effective \(K_d\) and concentration ratios (\(CR\)) determined using the new C-14 model;
- Calculation using the \(K_d\), \(CR\) and additional loss term from the top soil compartment determined using the new C-14 model.

\(^7\) For all calculations in this document, the SwiBAC version 1.1 was used.
The results are summarised in Tab. 10. The table shows that, introducing the new $K_d$ and $CR$ for C-14 alone results in an increase in BDCFs by about a factor of forty for both climate cases. Once the additional loss term from the top soil that are relevant for C-14 are included, the new C-14 model results in about a factor of four increase in the BDCF for the Temperate climate and an increase of about 4% for the Warm/Dry climate. The inclusion of additional C-14 losses from the top soil has a greater effect on the BDCF for the Warm/Dry climate because other losses from the surface soil are low relative to the Temperate case due to lower water fluxes (i.e. the additional rate of loss is more significant for the Warm/Dry case).

Tab. 10: Biosphere Dose Conversion Factors (BDCFs) Calculated with SwiBAC. BDCF given in $[Sv Bq^{-1}]$. 

<table>
<thead>
<tr>
<th>Calculation</th>
<th>Climate</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Temperate</td>
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<tr>
<td>SwiBAC</td>
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<tr>
<td>SwiBAC with $K_d$ and $CR$ from new C-14 model</td>
<td>3.1E-14</td>
</tr>
<tr>
<td>SwiBAC with $K_d$, $CR$ and additional loss term from new C-14 model</td>
<td>3.0E-15</td>
</tr>
</tbody>
</table>
8 Conclusions

A 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 BIOPROTA programme, notably through the explicit inclusion of a diffusive layer within the plant canopy.

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. The mass balance demonstrates the dominance of the flux of stable carbon through the upper part of the plant canopy and the atmospheric layer above the plant that is affected by advective movement of air (wind). Organic matter represents the major carbon pool within the top soil 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 (approximately hourly for soil gas and even faster for the diffusive and turbulent atmospheric layers around the plants).

Calculations with a unit source term of C-14 demonstrate a timescale of several hundred years to equilibrium, reflecting the turnover rate within the local aquifer. Uptake of C-14 by plants from the diffusive layer of the atmosphere dominates in comparison to either root uptake from the top soil or uptake from the turbulent layer of the atmosphere.

There is on-going discussion within the BIOPROTA forum regarding the appropriate way to represent the atmosphere within the plant canopy, in particular the boundary between turbulent mixing and diffusion dominated layers. In the absence of a consensus, the C-14 model presented herein adopts conservative assumptions that maximise the thickness of the diffusive layer and err on the side of calculating higher C-14 concentrations in the plants. Should C-14 become an important contributor to doses that approach regulatory thresholds, this area of the modelling should be revisited with a view to representing less conservative assumptions, which are supported by micrometeorological considerations.

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 different climate assumption have relatively little effect on the calculated results. The behaviour of C-14 in the more detailed C-14 model can be reproduced within SwiBAC by:

- calculating effective solid / liquid distribution coefficients, $K_d$, values for the soils and the local aquifer;
- introducing an additional loss term from the top soil to reflect losses to the atmosphere and crops; and
- calculating effective soil-to-plant concentration ratios for the different crops considered.

A $K_d$ value of 0.015 m$^3$ kg$^{-1}$ is appropriate for the deep soil and the local aquifer for all crop types. The $K_d$ for the top soil and the additional loss rate from the soil are dependent on the crop being modelled, with a difference of up to a factor of about five between crops. For the crops modelled in SwiBAC, the average effective $K_d$ for the top soil is 0.133 m$^3$ kg$^{-1}$ and the average additional loss rate from the top soil is 0.145 a$^{-1}$. Effective soil-to-plant concentration ratios vary from 1.6 for green vegetables to 17 for cereals for the cases studied.

The overall impact of the new C-14 model is to increase the BDCF for C-14 by about a factor of four for the Reference (Temperate) conditions considered in Nagra (2010). The BDCF for Warm/Dry conditions is increased by about 4%.
9 References


