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# In silico analysis of carbon stabilisation by plant and soil microbes for different weather scenarios

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**Abstract.** A plant's development is strongly linked to the water and carbon (C) flows in the soil-plant-atmosphere continuum. Ongoing climate shifts will alter the water and C cycles and affect plant phenotypes. Comprehensive models that simulate mechanistically and dynamically the feedback loops between water and C fluxes in the soil-plant system are useful tools to evaluate the sustainability of genotype-environment-management combinations that do not yet exist. In this study, we present the equations and implementation of a rhizosphere-soil model within the CPlantBox framework, a functional-structural plant model that represents plant processes and plant-soil interactions. The multi-scale plant-rhizosphere-soil coupling scheme previously used for CPlantBox was likewise updated, among others to include an implicit time-stepping. The model was implemented to simulate the effect of dry spells occurring at different plant development stages, and for different soil biokinetic parametrisations of microbial dynamics in soil. We could observe diverging results according to the date of occurrence of the dry spells and soil parametrisations. For instance, an earlier dry spell led to a lower cumulative plant C release, while later dry spells led to higher C input to the soil. For more reactive microbial communities, this higher C input caused a strong increase in $CO_2$ emissions, while, for the same weather scenario, we observed a lasting stabilisation of soil C with less reactive communities. This model can be used to gain insight into C and water flows at the plant scale, and the influence of soil-plant interactions on C cycling in soil.

## 1 Introduction

Understanding the dynamics driving the water and carbon (C) balances in the soil-plant-atmosphere continuum is key to predict, mitigate, and adapt agroecosystems to climate change (Silva and Lambers, 2021; George et al., 2024). While water plays an important role as a resource and as an intra- and inter-domain signalling carrier (De Swaef et al., 2022), C compounds can serve as an essential energy source or a biomass building block (Lynch et al., 2021; George et al., 2024).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


Plants link the water and C balances in the soil and atmosphere via plant-related processes, such as coupled stomatal regulation-photosynthesis-transpiration, C and water transport and storage in plant tissues, C usage (growth, maintenance, exudation) root-soil water exchanges and root C release (De Swaef et al., 2022; Lacointe and Minchin, 2019; Silva and Lambers, 2021). The plant's capacity to capture, transport and release water (resp. C) across domains (e.g., C fixation leading to rhizodeposit hotspots distribution (Landl et al., 2021a)) or within one domain (e.g., hydraulic lift, (Lynch et al., 2021)) is also strongly defined by the topology of its shoot (de la Fuente Cantó et al., 2020) and root system (Galindo-Castañeda et al., 2023; George et al., 2024; de la Fuente Cantó et al., 2020)–e.g., lateral root branching density, number of root tips (Lynch, 2021; Galindo-Castañeda et al., 2023). Likewise, plant anatomical characteristics (e.g., number and nature of the concentric root cells, number and size of the phloem and xylem vessels) strongly affect the flow within the plant (Lynch et al., 2021) and the plant-soil exchanges (Galindo-Castañeda et al., 2023; Lynch et al., 2021).

The quantity and quality of the C released by the plant influence the transfer of nutrients and energy to to the soil (de la Fuente Cantó et al., 2020) and thus microbial activity (Schnepf et al., 2022; Galindo-Castañeda et al., 2023, 2022; de la Fuente Cantó et al., 2020) directly as energy and biomass input and indirectly by changing the properties of the soil (Schnepf et al., 2022; de la Fuente Cantó et al., 2020; George et al., 2024). Root water uptake changes the soil moisture (Ruiz et al., 2021), which eventually triggers drought stress responses of soil microbial communities (Bardgett and Caruso, 2020). Plant-soil feedbacks drive inter and intra-specific plant interactions (Putten et al., 2013) (e.g., competition for soil resources). Plants can also exert direct feedback effects on themselves (e.g., aboveground-belowground feedback) which will influence their fitness. Those feedbacks depend on soil organic matter (SOM) content and texture, which determine soil water holding capacity and hence moisture availability under drought (Bardgett and Caruso, 2020; George et al., 2024).

Plant-soil exchanges lead to the creation of the rhizosphere, an area of soil around the root with biotic (rhizodeposition, microbial communities) and abiotic (structure, water content) characteristics distinctive from the bulk soil (George et al., 2024; de la Fuente Cantó et al., 2020). The hydraulic conductance of the rhizosphere is the primary constraint for plant water transport, especially in water-limited environments (De Swaef et al., 2022; Khare et al., 2022; Roose et al., 2016), leading to abiotic stress and stomatal closure (George et al., 2024; Damour et al., 2010) or better drought resilience in case of favorable abiotic conditions (Lynch et al., 2021).

The rhizosphere is also the most important hotspot of microbial activity on the planet (George et al., 2024; Lynch et al., 2021). Soil microbes control SOM decomposition and $CO_2$ release (Pagel et al., 2020) and regulate soil C allocation to the different organic and mineral pools. Rhizosphere microbes are relevant to soil C cycling as the activation-deactivation processes allow for rapid responses to the input of C and energy provided by rhizodeposits (George et al., 2024). Soil microbes are therefore a significant sink of photoassimilates, influencing root C release, root-to-shoot C allocation and overall plant growth (Lynch et al., 2021).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


Due to the tight coupling of water and C cycling between soil, microbes and plant, it becomes relevant to design integrated plant-microbiome traits adapted for specific soils to promote resource capture by plants and ensure the resilience of plant-soil systems to environmental stressors (Galindo-Castañeda et al., 2022; de la Fuente Cantó et al., 2020; Silva and Lambers, 2021). A thorough unterstanding of interactions between soil-microbes-plant (Galindo-Castañeda et al., 2022; Bardgett et al., 2013; Roose et al., 2016; George et al., 2024; Gaudio et al., 2021) that can lead to intra- and inter-specific competition (for light, water and nutrients), complementarity (spatio-temporal and niche processes) and facilitation (improving access to resources) is therefore essential to inform breeding choices (De Swaef et al., 2022; Gaudio et al., 2021).

Mechanistic biogeochemical modelling facilitates the analysis of complex systems (Schnepf et al., 2022; Putten et al., 2013). Especially Functional Structural Plant Models (FSPMs) link the plant structure with its function and simulate processes at the plant level (Schnepf et al., 2022; Ruiz et al., 2021). Coupling an FSPM with a soil model in a multiscale modelling framework leverages the strengths of different models and increase model accuracy (Schnepf et al., 2022; Roose et al., 2016; Gaudio et al., 2021). Small-scale models provide effective properties and predict emerging behaviour at higher scales, while models at coarser scales provide the initial and boundary conditions to the small scale models (Schnepf et al., 2022).

Although many studies looked at water and flow of (usually one) nutrient (especially phosphorus) in soil and rhizosphere (Mai et al., 2019; Ruiz et al., 2021; Roose et al., 2016), few focused on both water and C (Ruiz et al., 2021) and accounted for physiochemical processes (Pot et al., 2022). Moreover, many of the spatially explicit rhizosphere models ignore microorganisms (Roose et al., 2016) although the increasing resolution of those models make a detailed characterisation of the soil biochemistry more relevant (Roose et al., 2016; Lynch et al., 2021). FSPMs simulating C (Rees et al., 2020, 2023) and water flow were also developed (Lacointe and Minchin, 2019; Giraud et al., 2023) but simulating neither the soil C nor water flows (Lacointe and Minchin, 2019; Rees et al., 2020, 2023) or only the water flow (Giraud et al., 2023).

This study aimed to set up and implement a fully integrated plant-soil-microbiome model that accounts for root-microbiome interactions directly and enables the in-depth analysis of drought responses of C cycling in plant-soil systems. We present an extended version of the FSPM CPlantBox (Giraud et al., 2023). CPlantBox is a 3D functional structural full plant model and was used to model several processes across the plant, single root, ans pore scales (Mai et al., 2019; Landl et al., 2021a; Giraud et al., 2023). Root system simulations were also implemented to evaluate the effect of root system structure on the root-soil exchange of water (Khare et al., 2022), C (Landl et al., 2021a), or water and phosphorous (Mai et al., 2019). We coupled CPlantBox with TraiRhizo (Sırcan et al., 2025), a 1D axisymmetric soil model based. TraiRhizo offers a unique balance between complexity and precision for the C and microbial dynamic and a simplified representation of the soil structure (see review of Pot et al. (2022) for an evaluation of the analogous SpatC (Pagel et al., 2020) against other soil models). For this study, TraiRhizo was adapted and re-implemented in DuMu$^x$ (Koch et al., 2021) for a faster and more adaptable simulation setup. The two models were coupled using an updated version of the multiscale setup of Mai et al. (2019) to obtain higher accuracy and stability.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


In the first part of the paper, we present the equations of the model, with emphasis on the soil processes. We then present the scheme for the coupling of the different domains and modules. In the second section of the paper, we implement the model to evaluate how short dry spells at different stages of the plant's development affect the soil C balance and, in particular, the C stabilisation according to the biokinetic characteristics of the microbial community. In the last section of the paper, we discuss the output of the coupled model against experimental and *in silico* results, and we compare our framework against other existing simulation tools.

## 2 Material and methods

### 2.1 Overview of the multiscale framework

#### 2.1.1 Individual models

For the plant domain, we use the FSPM CPlantBox, as presented by Giraud et al. (2023). In CPlantBox, the plant is represented as a series of connected 1-dimensional segments, making a branched network of nodes in a 3-dimensional space (Fig. 1(a)). CPlantBox simulates the plant water flow using the analytical solution of (Meunier et al., 2017), and the coupled the stomatal regulation (Leuning, 1995) and FvCB-photosynthesis (Farquhar et al., 1980) models. The plant C balance is evaluated with a numerical solver (Lacointe and Minchin, 2019), which yields the semi-mechanistic plant growth rate.

For the soil domain, Sırcan et al. (2025) developed a 1-dimensional axisymmetric soil model that computes the C transport and microbial dynamics according to a set C release rate from a root segment. Their model was re-implemented within the existing soil framework of the FSPM (Mai et al., 2019) and adapted to take into account variations of water content. It was expanded to represent the 3-dimensional macroscale (Fig. 2) (Khare et al., 2022; Mai et al., 2019; Koch et al., 2021). The macroscale model is made of 3-dimensional sub-control volumes (i.e., voxels), while the microscale model is comprised of axisymmetric 1D sub-control volumes (i.e., segments). A list of the symbols of the soil models, their units and meanings can be found in appendix A. The explicitly represented soil C pools are: low molecular weight organic compounds (dissolved and sorbed), high molecular weight organic compounds, copiotrophic and oligotrophic microorganisms with active and dormant metabolic states, emitted $CO_2$ due to microbial respiration. In the following section, we give an overview of the spatial and temporal coupling of these models within a multiscale framework.

The hydraulic conductance of the soil–root interface is the primary constraint for plant water transport when the soil is dry. Achieving realistic results requires, therefore, high spatial resolution near the soil-root interface, leading to computationally expensive simulations (Roose et al., 2016; Khare et al., 2022). To balance computing speed and model accuracy, we therefore coupled the models presented in this section in a multiscale framework where the spatial resolution is set according to the distance from the soil-root interface.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 2.1.2 Spatial coupling

Figs. 1 and 2 give a graphical representation of the spatial coupling method, adapted from the approach presented by Mai et al. (2019) and Khare et al. (2022). Each root segment below-ground is allocated to a macroscale voxel, selected according to the location of the segment centre when it was first created. For each root segment, we initialise a microscale model that computes the water flow, C transport, and microbial dynamics based on the plant-soil water and C exchanges prescribed by the root segment. Other than in Sırcan et al. (2025), in which the plant-soil exchange was prescribed as boundary conditions at the root-soil interface, the net releases of water and C in this coupled model come from the simulation outputs of the FSPM, driven by inner plant flows and processes, such as photosynthesis, transpiration, and growth (Giraud et al., 2023).

The volume of the macroscale voxel is divided between the microscale domains it contains. Therefore, the maximum possible volume of a single microscale domain is the volume of the containing voxel. The total perirhizal volume around a root system (bulk soil) corresponds to the total volume of all the microscale domains. It is also equal to the sum of the volumes of all macroscale voxels containing at least one root segment. Therefore, the bulk soil volume depends on the root system structure and on the user-defined resolution at the macroscale rather than an *a priori* evaluation of the rhizosphere volume. The microbial reactions and adsorption are computed at the voxel scale for voxels that do not contain root segments. The biochemical reactions are computed at the microscale for voxels containing at least one segment. The resulting variation rates are represented at the macroscale as a sink term. The flow of water and transport of solutes between the voxels is computed at the macroscale and given as sink term to the microscale segments. Moreover, we scale the size of the microscale segments, meaning that the segments near the root surface are smaller than the ones further away. The macroscale domain is divided into subdomains whose concentrations and flows are computed in parallel while the microscale domains are distributed between processes run in parallel. The plant processes are not simulated in parallel.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


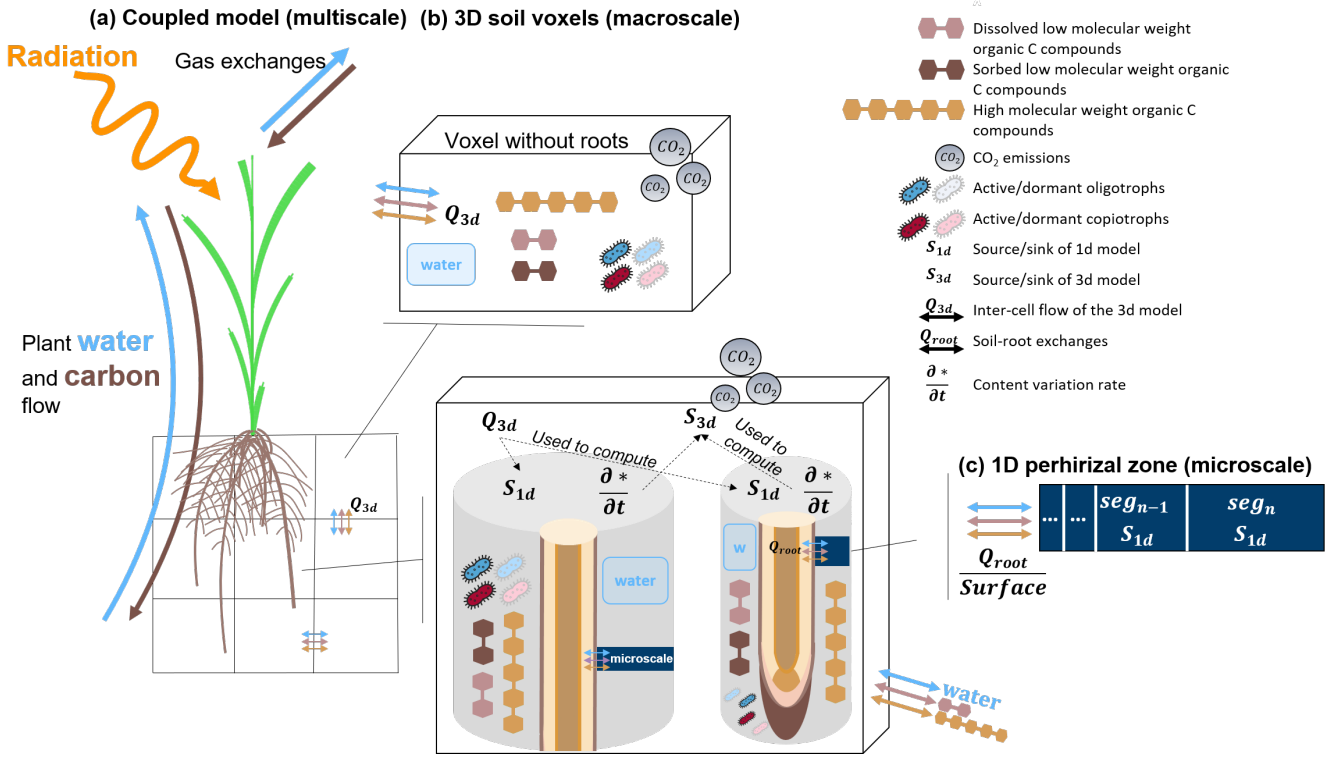


**Figure 1. Representation of the multiscale coupling** with (a) the whole multiscale model, (b) example of 3D macroscale soil voxels, (c) example of a 1D microscale model. The 3D soil model (black grid) is made up of 3D voxels (transparent rectangles with black borders). The 1D model is represented using the dark blue line in the 3D voxels. It lies between a root segment and the end of the implicitly-represented perirhizal zone (grey hollow cylinder).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


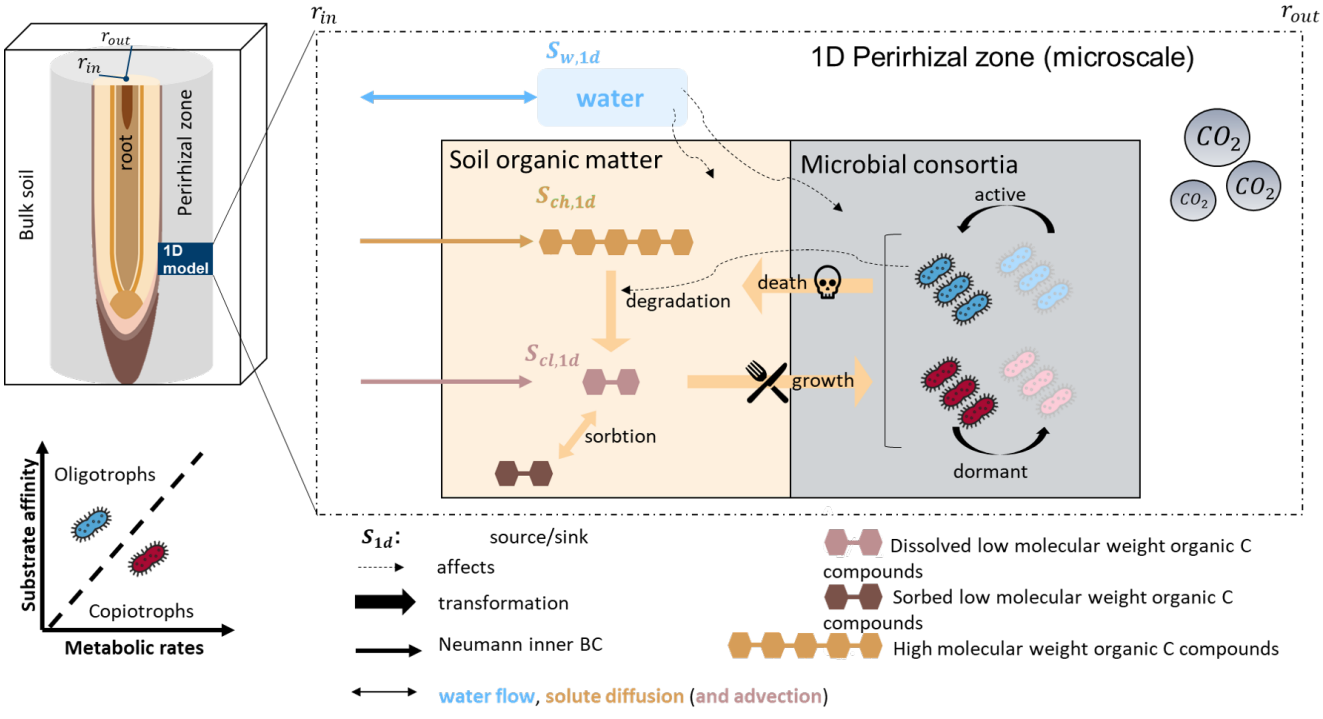


**Figure 2. Representation of the updated microscale model** (Sırcan et al., 2025) reimplemented within the multiscale framework (Mai et al., 2019; Koch et al., 2021). The model represents the soil domain around the root (perirhizal zone). Eight carbon pools are represented: carbon from organic compounds with a low molecular weight (dissolved and sorbed), organic compounds with a high molecular weight, active and dormant copiotrophs and oligotrophs, emitted microbial $CO_2$. Water flow and content are also represented. The graphic was adapted from Sırcan et al. (2025).

Fig. 3 gives a representation of the hard-coded direct interactions between the atmospheric conditions and the C and water pools represented in the plant and soil. For instance, for a set soil water content, high transpiration leads to a lower plant water potential and, thus, to a lower growth. In contrast, growth leads to a larger root system and leaf surface, allowing for higher transpiration. It is the interactions between those processes that drive the water and C balances of the overall system.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


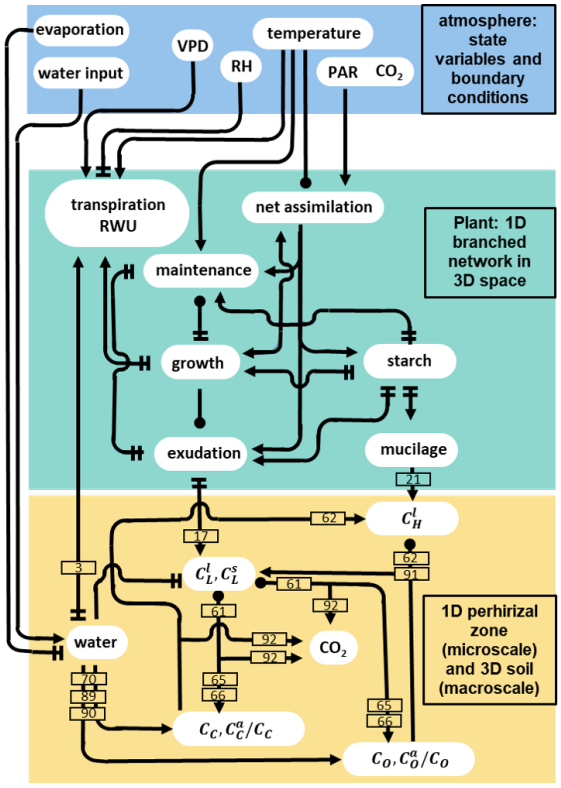


**Figure 3. Graphical representation of the direct interactions represented between the different carbon and water pools** plant model (green rectangle), soil models (yellow rectangle) and the atmospheric conditions given as input (blue rectangle). The lines ending with an arrow represent a positive effect, two perpendicular lines represent a negative effect, and a circle represents both a positive and negative effect (the net effect depends on the simulated conditions). The numbers in the rectangles give the indexes of the equations describing the corresponding process. The equations affecting the plant domain are defined in Giraud et al. (2023). The atmospheric conditions are represented by user-defined state variables and boundary conditions, e.g. vapour pressure deficit (VPD), relative humidity (RH), and incoming photosynthetically active radiations (PAR). Soil carbon pool data include the concentration of carbon from low molecular weight organic compounds in the soil and water phase (resp. $C_L^s$, $C_L^l$), high molecular weight organic compounds in the water phase ($C_H^l$), total or active copiotrophs (resp. $C_C$, $C_C^a$) and oligotrophs (resp. $C_O$, $C_O^a$).

### 2.1.3 Temporal coupling

The modules of the plant and soil models are implemented sequentially. The order of the implementation is presented in Fig. 4. Each "outer" loop (encompassing all the modules) represents one time-step. Within each time step, two nested fixed-point iterations are implemented:

1. the "first fixed point iteration" contains the interactions between the [a] soil water flow and solute transport (for the microscale and macroscale domains) and [b] plant water flow and stomatal regulation.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


2. the "second (inner) fixed point iteration" links the steady state plant water flow and stomatal regulation. This iteration loop was presented in Giraud et al. (2023) and will not be detailed further here.

These two nested iteration loops allow for a higher computing speed. Indeed, the inner fixed point iteration for the stomatal opening can necessitate several hundred iterations before convergence (especially in the case of water-induced stomatal closing). While the FcVB-stomatal regulation module can compute these iterations quickly, the code section evaluating the water flow at the macro- and microscale is much slower. Moreover, in the first iterations of the FcVB-stomatal computation, strong over- or under-estimation of the transpiration may occur, especially in case of sharp changes in environmental conditions. Using these inputs directly for soil flow computation could lead to non-convergence errors. Processes in the C and water cycles can operate on different timescales (Gaudio et al., 2021). Specifically, the speed of plant growth and phloem transport tends to be slower than the plant and soil water flow. When running a simulation, it may consequently be necessary to use a smaller time step within the fixed-point iteration. Thus, we set up an adaptive operator splitting between the outer time step and the first fixed-point iteration, with an automatic adaptation of the fixed-point iteration time step. Moreover, we used an implicit time stepping within the fixed-point iteration, which means that the output of the previous loop is used as initial and boundary conditions for the next loop of the iteration. This implicit time stepping is more stable than the explicit alternative and allows us to use larger time steps. Currently, the plant sucrose flow and growth are outside the iteration loop. Indeed, adding these modules to the fixed-point iteration would significantly slow the simulation. Also, for time steps $< 1\ h$, changes in plant shape and sucrose transport remain limited.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


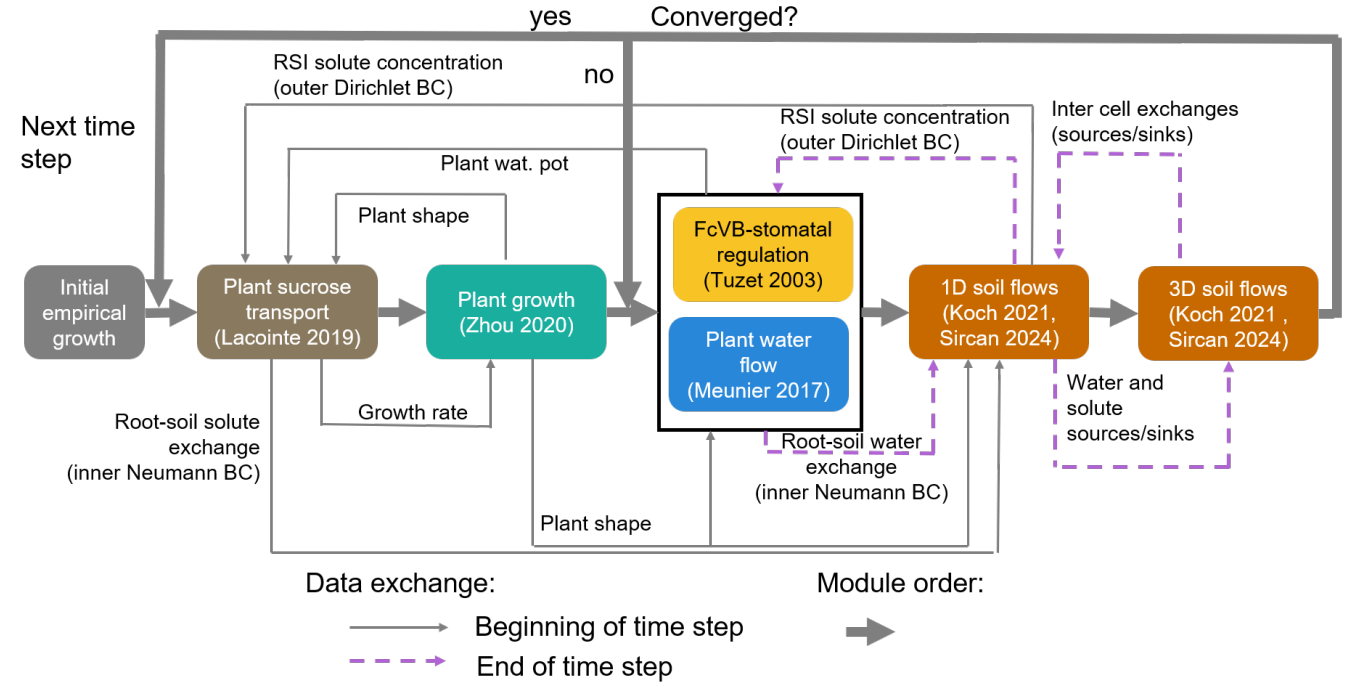


**Figure 4. Representation of the time loop**, as well as the implementation order and exchange of data between the modules. The loop including the soil flows (orange rectangles) corresponds to the outer iteration loop. The black rectangle outline containing the plant water flow (blue rectangle) and stomatal regulation (yellow rectangle) corresponds to the inner iteration loop. The plant sucrose transport and balance (brown rectangle) and growth (green rectangle) are not included in the iteration loop. Adapted from Giraud et al. (2023).

### 2.2 Governing Equations

These sections present the method used to simulate water and carbon turnover within the plant and the soil. Each section is divided between the plant-specific and soil-specific equations. For the soil part, the common equations for both the macro- and microscale are presented, followed by equations specific to each domain. The soil volume (volume of the solid and pores) is written in $cm^3$ $scv$ (sub-control volume). The amounts of solutes and microbes are given in units of equivalent carbon ($mol\ C$). As the equations describing the microbial reactions remain similar to those set up by Sırcan et al. (2025), these ordinary differential equations are included in appendix D.

#### 2.2.1 Plant water flow

The plant water model is described in Giraud et al. (2023). Briefly, we compute the plant xylem water flow as:

$$-K_{ax,x}\frac{\partial^2 \psi_{h,x}}{\partial^2 \xi} = -p_{seg} \times q_{w,plant-out} \text{ for } \Omega \backslash \partial\Omega, \quad (1)$$

$$\frac{\partial \psi_{h,x}}{\partial \xi} = 0 \text{ for } \partial\Omega \text{ (all organ end-nodes)} \quad (2)$$

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$K_{ax,x}$ ($cm^4\ hPa^{-1}d^{-1}$) is the xylem intrinsic axial conductance and $\xi$ ($cm$) is the local axial coordinate of the plant. $p_{seg}$ ($cm$) is the perimeter of the plant exchange zone, $\Omega$ the domain considered (here the plant), and $\partial\Omega$, the domain's boundary (here: the tip or end-node of each organ). We assume a no-flux boundary condition here as the plant-exterior water exchanges occur along the segments.

The net water sink is given by the lateral water flow ($q_{w,plant-out}$ in $cm\ d^{-1}$), which corresponds to the xylem-soil ($q_{w,root-soil}$) or xylem-atmosphere ($q_{w,leaf-air}$) water exchange:

$$q_{w,plant-out} = \begin{cases} q_{w,root-soil} = min(K_{lat,x}, K_{sri})(\psi_{h,x} - \psi_{m,1DS}) & \text{, if root} \\ q_{w,leaf-air} = K_{lat,min}(\psi_{h,x} - \psi_{h,ox}) & \text{, if leaf blade} \end{cases} \quad (3)$$

With $K_{lat,x}$ ($cm\ hPa^{-1}\ d^{-1}$) the lateral hydraulic conductivity of the root cortex (for roots) or of the vascular bundle-sheath (for leaves). $K_{sri}$ ($cm\ hPa^{-1}\ d^{-1}$) is the equivalent lateral hydraulic conductivity and $\psi_{m,1DS}$ ($hPa$) is the soil matric potential at the inner boundary of the corresponding 1D microscale soil domain (root-soil interface). $\psi_{h,ox}$ ($hPa$) is the water potential in the outer-xylem compartment, computed by the FvCB-stomatal regulation module. Note that, as changes in plant water storage are neglected, root water uptake equals transpiration at any given time step: $\sum_i^{segs} p_i q_{w,root-soil,i} = \sum_i^{nr} p_i q_{w,leaf-air,i}$, with $p_i$ ($cm$) the perimeter of the segment $i$ within the set $segs$.

$K_{sri}$ is computed from the soil and plant data:

$$K_{sri} = \begin{cases} \frac{K_{sat}\kappa_m(S_{sat})}{\Delta r_{root-1DS}} \text{ if } q_{w,root-soil} \leq 0 \\ \frac{K_{sat}}{\Delta r_{root-1DS}} \text{ else} \end{cases}, \quad (4)$$

$$K_{sat} = \frac{\kappa}{\mu_w} \quad (5)$$

With $K_{sat}$ ($cm\ hPa^{-1}\ d^{-1}$) the soil saturated hydraulic conductivity, $\mu_w$ ($hPa\ d$) the viscosity of the soil water solution, assumed equal to that of pure water at $20°C$. $\kappa$ ($cm^2$) is the intrinsic permeability of the soil and $\kappa_m$ ($-$) the relative conductivity loss, dependent on the soil water saturation ($S_{sat}$, $-$). $\Delta r_{root-1DS}$ ($cm$) is the distance in radial coordinate between the root surface and the centre of the inner segment of the microscale domain. Net root water release ($q_{w,root-soil} > 0$) is only limited by $K_{sat}$ in the soil, while net root water uptake ($q_{w,root-soil} < 0$) is also limited by $\kappa_m$.

### 2.2.2 Soil water flow

The variation in volumetric soil water content ($\theta$ in $cm^3\ water/cm^3\ scv$) is defined according to the Richards equations (Richards, 1931):

$$\frac{\partial\theta}{\partial t} = \nabla \cdot (K(S_{sat})(\nabla\psi_{m,XDS} - \nabla\psi_{g,XDS})) + S_\theta \quad (6)$$

With $K(S_{sat})$ ($cm^2\ hPa^{-1}\ d^{-1}$) the unsaturated hydraulic conductivity (hereafter written as $K$ for simplicity), $\nabla\psi_{m,XDS}$ and $\nabla\psi_{g,XDS}$ ($hPa/cm$) are the gradients of matric and gravitational water potentials in either the macroscale ($\psi_{3DS}$) or microscale ($\psi_{1DS}$) domain, respectively.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$S_\theta$ ($cm^3\ water\ cm^{-3}\ scv\ d^{-1}$) is the net source of water in the domain. $\nabla$ is the nabla operator, either for the 1D axisymmetric (radial derivative $\frac{\partial}{\partial r}$) or for the 3D domain ($\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$). We moreover have:

$$\theta = \phi S_{sat} \tag{7}$$

with $\phi$ ($cm^3\ pore/cm^3\ scv$) the soil porosity (assumed constant). for simplicity, we assume that $\phi = \theta_s$, with $\theta_s$ ($cm^3\ water/cm^3\ scv$) the $\theta$ value at saturation. $\theta_r$ ($cm^3\ water/cm^3\ scv$) is the lowest possible $\theta$ value (residual water content). The hydraulic conductivity is defined using the pore size distribution model of Mualem (1976) and the water retention function is computed according to van Genuchten (1980):

$$S_{sat} = \left(\frac{1}{1 + (\alpha\ \psi_{c,XDS})^n}\right)^{1-1/n} \tag{8}$$

$$\psi_{c,XDS} = \psi_{n,XDS} - \psi_{m,XDS} \tag{9}$$

$$K = \kappa_m(S_{sat}) K_{sat} \tag{10}$$

$$\kappa_m(S_{sat}) = S_{sat}^{l_{soil}} \times [1 - (1 - (S_{sat})^{n/(n-1)})^{1-1/n}]^2 \tag{11}$$

$\psi_n$ ($hPa$) is the reference pressure, set to 1000 $hPa$, and $\psi_c$ ($hPa$) is the capillary pressure. $\alpha$ ($cm^{-1}$) is related to the inverse of the air entry suction, $n$ ($-$) is a shape parameter, $l_{soil}$ ($-$) is the soil tortuosity. The implementation of Eq. (6) for the macroscale 3D soil and microscale 1D soil are given respectively in appendices B1 and B2.

### 2.2.3 Plant carbon transport

The plant sucrose model used for this study is based on the one presented by Giraud et al. (2023). The model was adapted to simulate mucilage release. The variation of sucrose-carbon concentration in the sieve tube ($C_L^{st}$ in $mol\ C\ cm^{-3}\ st\ d^{-1}$, with $cm^3\ st$ the sieve tube volume) is computed from Eq. (12):

$$\frac{\partial C_L^{st}}{\partial t} + \frac{\partial}{\partial \xi}\left(C_L^{st} \times K_{ax,st}(RT_{seg}\frac{\partial C_L^{st}}{\partial \xi} + \frac{\partial \psi_{h,x}}{\partial \xi} + \frac{\partial \psi_{g,x}}{\partial \xi})\right) - S_{exud,st} - S_{starch,st} - S_{other,st} = 0 \quad \text{for } \Omega \backslash \partial\Omega,\ t > t_0, \tag{12}$$

$$K_{ax,st}(RT_{seg}\frac{\partial C_L^{st}}{\partial \xi} + \frac{\partial \psi_{h,x}}{\partial \xi} + \frac{\partial \psi_{g,x}}{\partial \xi}) = 0 \quad \text{for } \partial\Omega \tag{13}$$

$$C_L^{st} = C_{L,0}^{st} \quad \text{for } t = t_0, \tag{14}$$

With $R$ ($hPa\ cm^3\ K^{-1}\ mol^{-1}$) the ideal gas constant, $K_{ax,st}$ ($cm^4\ hPa^{-1} d^{-1}$) the sieve tube axial intrinsic conductance, $T_{seg}$ ($K$) the temperature of the plant segment. $S_{exud,st}$ ($mol\ cm^{-3}\ st\ d^{-1}$) is the loss of $C_L^{st}$ by exudation of low molecular weight organic carbon compounds, $S_{starch}$ ($mol\ cm^{-3}\ st\ d^{-1}$) is the loss or gain of $C_L^{st}$ by starch synthesis or degradation, $S_{other,st}$ ($mol\ cm^{-3}\ st\ d^{-1}$) represents other net sinks of $C_L^{st}$–like gain by assimilation and inflow from the mesophyll

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


compartment.

We assume that the exudation of low molecular weight organic carbon occurs via a passive diffusion (Rakshit et al., 2021; Ma et al., 2022), represented by a mass transfer approach:

$$S_{exud,st} = q_{exud} \frac{2\pi\ r_{in}\ L}{V_{st}} \tag{15}$$

$$q_{exud} = K_{lat,st}\ (C_L^{st} - C_L^l) \tag{16}$$

With $K_{lat,st}$ $(cm\ d^{-1})$ is the lateral sieve tube conductivity for sucrose, $V_{st}$ $(cm^3\ st)$ is the sieve tube volume. We assume that exudation occurs mainly near the root tip (Rakshit et al., 2021; Badri and Vivanco, 2009; Neumann and Römheld, 2009). Therefore, $K_{lat,st} > 0$ only for the last segment of growing roots. $C_L^l$ $(mol\ C/cm^3 water)$ corresponds to the concentration of dissolved low molecular weight organic carbon in the soil water at the root-soil interface. It is obtained from the inner segment of the microscale soil domain assigned to the root segment. We assume that the mucilage is made from starch (*starch*, in $mol\ C/cm^3$) before being released via an active process (Rougier, 1981; Nguyen, 2009; Kutschera-Mitter et al., 1998). The production and release processes are represented in the following equations:

$$\frac{\partial starch}{\partial t} = S_{starch,st} - S_{mucil,st} \tag{17}$$

$$S_{starch,st} = k_{targ,starch}(C_L^{st} - C_{L,targ}^{st}) \tag{18}$$

$$S_{mucil,st} = q_{mucil} \frac{2\pi\ r_{in}\ L_i}{V_{st}} \tag{19}$$

$$q_{mucil} = k_{mucil} starch \tag{20}$$

With $k_{targ,starch}$ $(1/d)$ and $k_{mucil}$ $(cm/d)$ parameters controlling respectively the synthesis and decay rate of starch and the release of mucilage. $C_{L,targ,st}^l$ defines the target $C_L^{st}$ and thus the threshold between starch synthesis and desynthesis. As in Hirschberg et al. (1998), the release of mucilage is represented via a simple first-order kinetic. We then obtain $S_{mucil}$ $(mol\ cm^{-3}\ st\ d^{-1})$, the release rate of mucilage. $k_{mucil} > 0$ only at the tip (in our model: the last segment) of growing roots. Both $q_{exud}$ and $q_{mucil}$ $(mol\ cm^{-2}\ d^{-1})$ can then be used by the microscale soil domains (see Eq. (C13), Eq. (C17)).

### 2.2.4 Soil carbon transport

The changes in solute concentration are computed using the advection-diffusion-reaction equation—see Ahusborde et al. (2015) and Helmig (1997, Eq 3.100):

$$\frac{\partial \theta C_X^l}{\partial t} - \nabla \cdot \left(C_X^l \boldsymbol{u}_X\right) - \nabla \cdot (D_X(\theta,\phi)\nabla C_X^l) - S_X\ (-S_{1DS-3DS,X}) = 0 \tag{21}$$

$$S_{ads,X} + S_{microbe,X} = S_X \tag{22}$$

$C_X^l$ $(mol/cm^3\ water)$ is either the concentration of carbon from dissolved low molecular weight organic compounds ($C_L^l$) or high molecular weight organic compounds ($C_H^l$) in the soil liquid solution. $S_X$ $(mol\ C\ cm^{-3}\ scv\ d^{-1})$ is the net source of $C_X^l$, and it encompasses the adsorption of $C_X^l$ ($S_{ads,X}$, $mol\ C\ cm^{-3}\ scv\ d^{-1}$, see section 2.2.5) and the changes caused by microbial reactions ($S_{microbe,X}$, $mol\ C\ cm^{-3}\ scv\ d^{-1}$, see appendix D and Eq. (C1)). $S_{1DS-3DS,X}$ is an additional source term only used at the microscale and presented in Eq. (C7). $\boldsymbol{u}_X$ is the advective flux.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$D_X(\theta,\phi)$, the effective dispersion in the porous medium (caused by molecular diffusion and hydrodynamic dispersion), is obtained from Millington and Quirk (1961), as implemented by Koch et al. (2021):

$$D_X(\theta,\phi) = D_{Xw}\frac{\theta^{\frac{10}{3}}}{\phi^2} \tag{23}$$

With $D_{Xw}$ $(cm^2/d)$ the diffusion coefficient of the carbon compound in water. Low molecular weight organic C compounds can be modelled as true solutes and are thus subject to convection. High molecular weight carbon compounds correspond to the plant mucilage releases, a gel-like substance when hydrated (Ma et al., 2022; Kutschera-Mitter et al., 1998). To simulate the rheology of mucilage slime, we adopt a simplified approach with a null advective flux ($\boldsymbol{u}_H$) and a lower diffusion coefficient ($D_{H,w} < D_{L,w}$). The implementation of Eq. (21) for the macroscale 3D soil and microscale 1D soil are given respectively in appendices C1 and C2.

### 2.2.5 Adsorption

We describe in this section the adsorption of low molecular weight organic C compounds ($C_L$) from the liquid phase ($C_L^l$) onto the solid phase ($C_L^s$). As Sırcan et al. (2025), we describe the adsorption as linear. However, instead of equilibrium sorption, we used linear first-order kinetics. This was necessary in order to obtain the same result at the micro- and the macroscale. Moreover, not assuming instantaneous equilibrium allows us to set lower time steps during the simulations. We further assume that only the low molecular weight organic substances can be sorbed. Adsorption was implemented according to Ahrens et al. (2020):

$$\frac{\partial C_L^s}{\partial t} = k_{ads}C_L^l(C_{L,max}^s - C_L^s) - k_{des}C_L^s \tag{24}$$

$$C_{L,max}^s = C_{L,max}^s = \rho_b\frac{k_{clsmax}\ k_{clay+<20\mu msilt}}{M_{mass,C}} \tag{25}$$

with $k_{ads}$ ($23265.14\ cm^3\ scv\ mol^{-1}\ C\ d^{-1}$) and $k_{des}$ ($4.47\ d^{-1}$) the adsorption and desorption rates, defined according to the values given by Ahrens et al. (2020). $C_{L,max}^s$ ($mol\ C\ cm^3\ scv$) is the maximal concentration of adsorbed $C_L^s$, $\rho_b$ ($1.51\ g$ mineral soil$/cm^3\ scv$) is the soil bulk density, $M_{mass,C}$ ($12.011\ g\ C\ mol^{-1}\ C$ ) is the molar mass of carbon, $k_{clay+<20\mu msilt}$ ($0.45-$, Wang et al. (2018)) is the fraction of clay and silt smaller than $20\ \mu m$. $k_{cssmax}$ $(-)$ is an empirical factor defined according to the make up of the clay minerals in the soil. According to Jiang et al. (2014), the Selhausen soil (used to calibrate the model) is dominated by illites, a $2:1$ mineral. Consequently, $k_{cssmax} = 0.079$ (Ahrens et al., 2020). This yields $C_{L,max}^s = 4.5e^{-3}\ mol\ C\ cm^{-3}\ scv$). From the adsorption dynamic, we get the adsorption net sink for dissolved low molecular weight organic carbon: $S_{ads,L} = -\frac{\partial C_L^s}{\partial t}$, used in Eq. (22). As high molecular weight organic carbon compounds represent the mucilage gel, no adsorption is represented: $S_{ads,H} = 0$.

### 2.2.6 Plant growth and perirhizal zone

We simulate dynamic plants that grow according to input parameters (representing plants genetically determined characteristics) and to their water and sucrose status (see Giraud et al. (2023)). This leads to changes in root segment lengths and to the creation

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


of new root segments. The method used to define the shape, water and solute content of new or growing microscale domains is presented below.

Currently, each root segment (and associated microscale domain) is allocated to the soil voxel containing its centre when the segment is first created, even if one or both segment extremities are out of the voxel. In order for the output to be realistic, it is therefore important for the maximum root segment size to be lower or near the length of a soil voxel. Moreover, for the current setup, root segments will remain in the same soil voxel even if the centre of an existing segment (because of segment elongation) moves to another voxel. We assume that these simplifications will have a limited influence on the results if the resolution is high enough. After simulating plant growth for the time step $N$, we obtain the new lengths ($L$, $cm$) and radius ($r_{in}$, $cm$) of the roots, which are, respectively, the lengths and inner boundary of the microscale domains. From these shape data, we recompute the outer radial boundary of the 1D domains ($r_{out}$, $cm$) according to the volume of the soil voxels ($V_{3DS,scv}$) and the number of microscale domains contained within ($nr$). For the microscale domain $k$ in the voxel $i$:

$$r_{out,k}^{N} = \sqrt{\frac{r_{in,k}^2 \, L_k^N}{\sum_j^{nr_{i,N}} r_{in,j}^2 \, L_j^N} \frac{V_{3DS}}{\pi \, L_k^N} + r_{in,k}^2} \tag{26}$$

Consequently, creation of new roots or changes in $L$ and $r_{in}$ of existing roots in a voxel can lead to changes in the perirhizal zone volume allocated to an individual microscale soil domain. From the soil point of view, a higher density of roots in the voxel leads to smaller perirhizal zones for each of the root segments contained in it. The description of the method used to update the amounts of water and carbon in the microscale models as they are created and change shape is presented in the appendix E. In brief, the gradient of existing 1D domains with decreasing volume is preserved. We then compute the volume of newly freed soil for each voxel. From the amount of water and carbon lost by the 1D models, we obtain the mean water content and carbon concentration in the freed space. This volume (and corresponding water and solute contents) is distributed between the new and expanding microscale domains to respect the results of Eq. (26).

### 2.3 Model application: The effect of dry spells on soil carbon and microbial dynamics near a growing plant

The implementation setup for the coupled model follows the one used in Giraud et al. (2023), with Van Genuchten parameters measured from one testing site of the Research Center Jülich, located in Selhausen (50.8659 N, 6.4471 E). We simulated the growth of a C3 monocot under a control scenario (hereafter called *baseline*) and compared it with dry spells at two plant development stages. Both dry spells were represented by a period of one week without rainfall: 11 to 18 days and 18 to 25 days after sowing, hereafter called *earlyDry* and *lateDry*. The virtual plants were obtained by running the plant model up to day 10 (after sowing) using a mean empirical growth rate (neither dependent on the carbon- nor water-flow) and without simulation of the water and carbon fluxes. From the $10^{th}$ day onward, we simulated the carbon and water fluxes and of the carbon- and water-limited growth, as well as the soil carbon dynamic. The plants all grew under the *baseline* conditions with a static soil (constant mean $\psi_{m,soil} = -100$ $cm$ at hydraulic equilibrium), except during the dry spells: day of growth 11 to 18 for *earlyDry*, and 18 to 25 for *lateDry*). At the start of the dry spells, the mean soil water potential was lowered to $-450$ $cm$ and warmer and drier atmospheric conditions were simulated. After the dry spells, the *baseline* environmental and static soil

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


water conditions were used. We used a no-flux boundary condition for the macroscale soil. Fig. 5 summarises the timeline of the three scenarios.

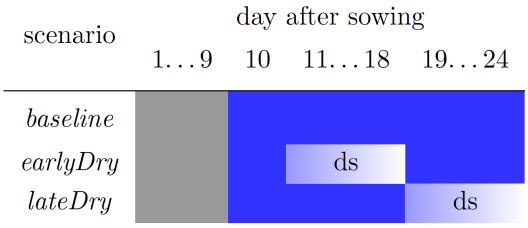


**Figure 5. Timeline of the simulations.** The grey (resp. blue) cells indicate the empirical (resp. semi-mechanistic) growth period and "ds" the implementation of the dynamic soil. The blue gradient during the dynamic soil simulation represents the decreasing soil water content. The sharp shift from dark to light (resp. light to dark) blue at the beginning (resp. end) of the dry spells represents the implementation of the *dry spell* (resp. *baseline*) atmospheric and initial (resp. constant) soil variables. Figure taken from Giraud et al. (2023)

For the plant model, the calibration of Giraud et al. (2023) was adapted to better follow our assumptions regarding the plant mucilage and carbon dynamic (e.g., preferential carbon usage for growth over exudation), and to address the divergences between the outputs of Giraud et al. (2023) and experimental observation (light dry spells caused carbon rather than water scarcity). Changes were also made to the lateral conductivity ($k_{lat,x}$, $cm\ hPa^{-1}\ d^{-1}$) in the mature root zone: the constant value was computed according to Bramley et al. (2007, Fig. 4.15) and set to $1.5\%$ of $k_{lat,x}$ within the immature root zone, see appendix H for a more detailed description.

The selection of the biokinetic parameter sets is given in appendix I. Briefly, Sırcan et al. (2025) computed 1650 parameter sets respecting parameter and process constraints defined according to a literature review. Those sets were divided into three groups according to the resulting $C_L^l$ radial profile for the microscale domains. 33 sets were selected randomly from each group and a simulation was run for four days. We then selected three parameter sets giving diverging results. Table 1 presents the characteristics of the selected sets. The first set, thereafter called *highCO2*, led to a high $CO_2$ production in spite of a low microbial development. The second set, thereafter called *highMB*, led to the highest microbial development. The third set, thereafter called *lowMUptake*, led to the highest soil solute concentration (low microbial solute uptake).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


**Table 1.** Qualitative summary of the characteristics of the three selected biokinetic parameter sets (*highCO2*, *highMB*, *lowMUptake*). O: oligotrophs, C: copiotrophs, (de)act.: activation and deactivation, *VS*: compared against. The evaluation has the following order (representing the low-to-high gradient): $- < . < + < ++$

| **denomination** | **fitness** | | **act. *VS* deact.** | | **(de)act. *VS* growth + decay** | | **O *VS* C** | | **$CO_2$ losses** |
|---|---|---|---|---|---|---|---|---|---|
| | **O** | **C** | **O** | **C** | **O** | **C** | **(de)act.** | **fitness** | |
| *highCO2* | + | – | . | . | + | + | . | + | ++ |
| *highMB* | + | . | + | + | ++ | . | – | + | + |
| *lowMUptake* | – | . | – | – | . | . | . | – | - |

### 2.4 Analysis of the outputs

The data were treated and visualised with Python3.10 (Van Rossum and Drake Jr, 1995).

#### 2.4.1 Scale definition for model evaluation

To take advantage of the multiscale setup, we evaluated the model outputs at four different scales: macroscale, bulk soil, perirhizal$_{trunc}$, microscale. We define the macroscale as the soil voxels (Fig. 1(b)) that contain at least one root at the end of the simulations in any of the scenarios. This soil space is therefore constant and equal for all the simulations. We define the bulk soil as the macroscale data of voxels containing at least one root at each time step, potentially different for each simulation. For the perirhizal$_{trunc}$ analysis, we aggregated the mean concentrations for each microscale domain truncated at a specified distance from the root surface, denoted as $\Delta r_{analysis}$. The value of $\Delta r_{analysis}$ was pragmatically set to $0.06\ cm$. It corresponds to the minimum distance between the inner and outer boundaries of the microscale domains obtained during the simulation. By setting a consistent distance between the inner and outer boundaries of the truncated domains, we obtained a partial uniformity between the domains that reduced variations that could arise from differences in soil allocation to each domain (see Eq. (26)). Moreover, using these truncated 1D models allowed us to evaluate a soil area nearer to the root surface, for comparison with the bulk soil scale. At the microscale, we evaluated the data for each segment of the 1D models (Fig. 1(c)) individually.

#### 2.4.2 Vertical concentration profiles

To evaluate the vertical concentration profiles, we computed the total soil volume, water volume, and C content (for each C pool) for each depth at the bulk soil scale. This allowed us to determine the corresponding mean C concentration and water content around the root systems. Additionally, we present the minimum and maximum C concentrations (for each C pool) and water content values at each soil depth to capture the lateral variability.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 2.4.3 Complementary cumulative volume distributions

We created complementary cumulative volume distribution plots of the concentration at the perirhizal$_{trunc}$ scale. In these plots, the x-axis represents different concentration values. The y-axis shows the absolute or relative volume of the selected perirhizal zone (up to $0.06\ cm$ from the root surface) with concentrations equal to or greater than the corresponding x-axis value. This representation provides insight into the spatial variability and distribution of concentrations within the specified zone. Additionally, these graphs allow us to evaluate how much of the perirhizal zone volume exceeds certain concentration levels, such as hotspot thresholds.

### 2.4.4 Relative change of soil carbon distribution

To evaluate the change in plant-soil C turnover for the different weather scenarios and biokinetic parameter sets, we categorised C into four pools: solutes (dissolved and sorbed low molecular weight organic C and high molecular weight organic C), microbes (including total oligotrophic and copiotrophic C), active microbes (including active oligotrophic and copiotrophic C), and emitted $CO_2$ (microbial respiration). We evaluated the C content at the macroscale for each of these pools at each time step and normalised the values for *earlyDry* and *lateDry* under each biokinetic parameter set according to the corresponding baseline scenario: $(C_{X,spell} - C_{X,baseline})/C_{X,baseline}$, with $X$ the name of the C pool.

### 2.4.5 Soil organic carbon hotspots

One important effect of plant C releases is the resulting changes in soil organic C (SOC). Using the study of Poeplau and Don (2023), we set three SOC thresholds defined according to the $SOC/SOC_{expected}$ ratio: 0.65, 0.83, 1.16. $SOC_{expected}$ ($mol\ C\ cm^3\ scv$) is the average expected SOC according to the soil clay content. Following the method of Poeplau and Don (2023) and the Selhausen clay content data of Wang et al. (2018), we set $SOC_{expected} = \frac{\rho_b}{1000 M_C}(0.0288 k_{clay} + 13.674) = 2.36e^{-3}\ mol\ C\ cm^3\ scv$, with $k_{clay}$ the soil clay content in $g\ kg^{-1}$, $\rho_b$ ($g/cm^3\ scv$) the soil bulk density, $M_C$ ($g\ C/mol\ C$) the C molar mass. The $1/1000$ factor is used to go from $g\ kg^{-1}$ to $g\ g^{-1}$.

A first evaluation of the outputs showed that our simulated values were almost always in the lowest SOC class and significantly below the mean Selhausen SOC reported by Wang et al. (2018). For the hotspot analysis, we therefore added an $SOC_{slow}$ class representing the very slow decomposing SOC, assumed to be constant over the study period. We set $SOC_{slow} = SOC_{theoric} - SOC_{simulated,init}$, with $SOC_{simulated,init}$ the total SOC explicitly simulated in our model (solute and microbial pools) at the beginning of the simulation, and $SOC_{theoric}$ the value from Wang et al. (2018). We then set the variable $SOC = SOC_{simulated} + SOC_{slow}$, computed at the microscale. This is the value used to compare with the SOC thresholds given by Poeplau and Don (2023). We use a stacked area graph to represent the SOC hotspots, as soil above the higher thresholds is also above the lower thresholds. As presented by Landl et al. (2021a), we computed the volume-normalised hotspot volume to obtain a metric for the efficiency of the rhizodeposition.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


#### 2.4.6 Radial concentration profiles

Finally, for the microscale, we presented C concentration data for all segments of the 1D domains on one scatter plot per weather scenario and parameter set, giving, on the x-axis, the radial coordinate of the segment centers according to the root surface.

## 3 Results

### 3.1 Three-dimensional simulation of microbial carbon dynamics in the soil-plant system

The integrated plant-soil-microbiome model extends the FSPM model of Giraud et al. (2023)) by implementing microbial carbon (C) dynamics in soil. Consequently, the extended FSPM model now provides 3D simulations of plant architecture, water and C dynamics in the plant and the soil, and microbial dynamics in the soil, including the rhizosphere. While this study focuses on C cycling and microbial dynamics at the root-soil interface, more detailed simulation results regarding water and C flow in a plant for the three considered weather scenarios are given in Giraud et al. (2023). Fig. 6 shows a typical simulation after 24.5d of plant growth (midday) for a biokinetic parameterisation that results in high microbial $CO_2$ production (*highCO2*) under the *baseline* scenario. The simulation highlights an increasing concentration of dissolved low molecular weight organic C ($C_L^l$) and active copiotrophs ($C_C^a$) in response to root exudation in the upper part of the root system, near its centre.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


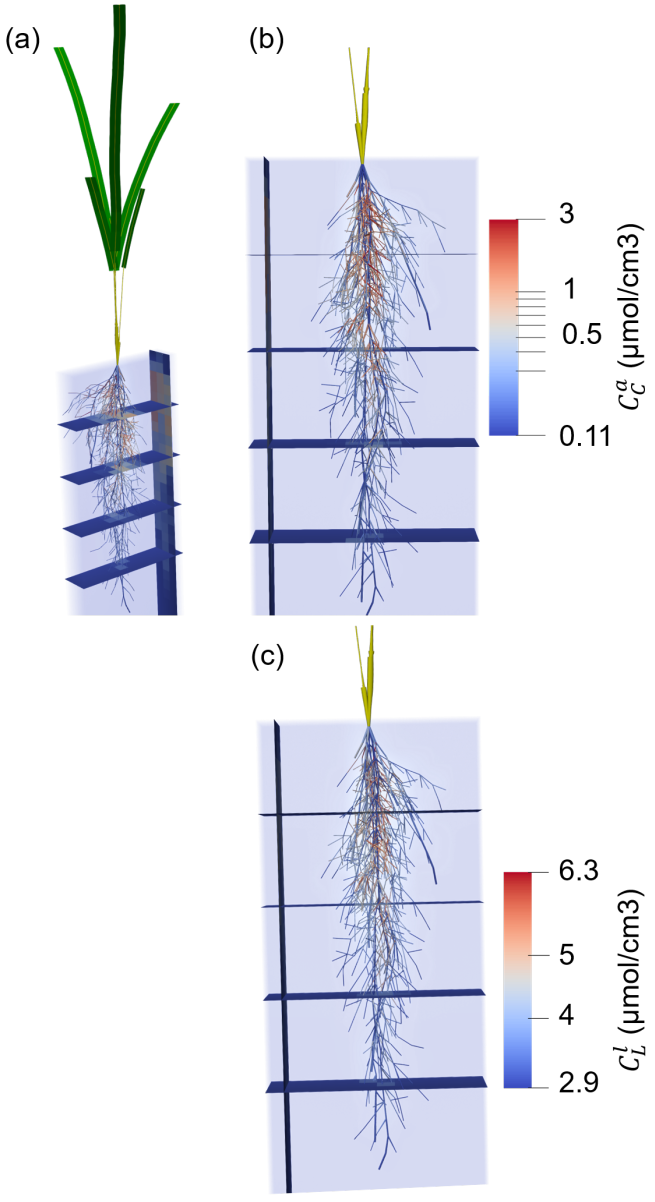


**Figure 6. 3D representation of the plant and soil domains** for microbial biokinetic parameterisation *highCO2* under the *baseline* scenario at 24.5d of growth, with (**A**) the whole plant, (**B**, **C**) zoom on the root system. (**A**, **B**) present the concentration of active copiotrophic biomass C ($C_C^a$) and (**C**) that of dissolved low molecular weight organic C ($C_L^l$). The soil colours give the concentration in the bulk soil. The root colours give the concentration at the soil-root interface. Unified colours were given to the aboveground roots, shoot segments and leaf blades.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 3.2 Plant processes

Fig. 7.A presents the plant xylem mean water potential ($\psi_x$, $cm$) for each biokinetic parameterisation and weather scenario. The simulation results reflect the diurnal dynamics of $\psi_x$ in response to the truncated sinusoidal curve used to describe the atmospheric conditions (light input, air relative humidity and temperature). These boundary conditions affected the plant stomatal regulation and, thus, the C assimilation and transpiration rate. We observed an increase of $\psi_x$ over time for *baseline* as the leaf:root ratio decreased. With drought, $\psi_x$ rapidly decreased at the beginning of the dry spells and recovered after its end in response to changes in soil water content and mean air relative humidity during the dry spells (see (Giraud et al., 2023, Table 1)). Towards the end of the simulation with *earlyDry*, $\psi_x$ converged to the values of *baseline*, indicating a full recovery of the plant water uptake capacity. As a consequence of the lower leaf:root ratio, $\psi_x$ was lower at the beginning of the dry spells for *earlyDry* ($11^{th}$ day) than for *lateDry* ($18^{th}$ day). However, in comparison to *earlyDry*, the higher plant transpiration under *lateDry* with higher total leaf and root surface area led to a quicker decrease in soil water content. This mechanism induced lower $\psi_x$ in the *lateDry* compared to the *earlyDry* scenario from the third day after the start of the dry spells onward ($13^{th}$ and $20^{th}$ day).

Fig. 7.B shows the cumulative amount of C used for growth (and growth respiration) during the simulation. The diurnal cycle of $\psi_x$ affected the plant growth. During the day, the transpiration-induced lower $\psi_x$ limited plant growth compared to the night, where increased $\psi_x$ permitted faster, albeit still water-limited, C assimilation and biomass production. The required C was taken from the starch reserves built up during the day. We can also observe trends over the simulation. Unlike younger plants, older plants could maintain growth during the diurnal period outside of the dry spells. During the dry spells, growth occurred only at night and at a severely reduced rate. On the last three nights of the late dry spell, we observed no night-growth due to lower plant night $\psi_x$.

Plant maintenance respiration increased during the spells due to the higher air temperatures. In the *earlyDry* scenario, plant growth was severely limited compared to *baseline*, resulting in a lower plant maintenance respiration rate after the dry spell ended ($18^{th}$ day). For *lateDry*, we saw a lower maintenance respiration rate from the fourth day of the spell. The total cumulative respiration (growth and maintenance related) at the end of the simulation was highest for the *baseline* scenario. It was about $29\%$ lower for *earlyDry* and $18\%$ lower for *lateDry*. The biokinetic parameterisation had no significant effect on the plant water processes or growth and maintenance.

Figs 7.C and D present the cumulative amount of C used for (respectivelly) passive exudation and active mucilage release during the simulation. The plant water balance affected the exudation rate. During the simulation, exudation occurred only under limited C use for growth in response to low $\psi_x$. Although the mucilage release was not always maintained at night (e.g., at the end of the *earlyDry* simulation), this process was less affected by the diurnal cycle than the exudation. This led to qualitative changes in the type of C released by the plant throughout the day. In comparison to *baseline* the early dry spell led to a lower total exudation at the end of the simulation: $-32\%$, $-35\%$, and $-37\%$ for *highCO2*, *highMB*, and *lowMUptake*, respectively. Conversely, the late dry spell resulted in higher exudation compared to *baseline*: $+29\%$ for *highCO2* and *highMB*, $+26\%$ for *lowMUptake*. Thus, the dry spells triggered both positive and negative effects on exudation. On the one hand, more

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$C$ became available for exudation with decreasing plant growth. On the other hand, the lower $\psi_x$ led to a closing of the stomata, causing a lower assimilation rate per unit of leaf area.

Lower plant growth also led to lower leaf and total root surface area compared to *baseline*, which limited exudation. The effect of the simulated spells on total exudation was, therefore, dependent on the stage of plant growth at the start of the spell. After the end of the early dry spell (days 18-23), the daily plant exudation for *earlyDry* was higher than for *baseline*, partially reducing the exudation gap between the two. The total mucilage release under *earlyDry* at the end of the simulation was close to that under *baseline*: $-11\%$, $-2\%$, and $+6\%$ for parameter sets *highCO2*, *highMB*, and *lowMUptake*, respectively. In contrast, mucilage release reached $+139\%$ for *highCO2* and *highMB* and $+170\%$ for *lowMUptake* under *lateDry*. We found an effect of the biokinetic parameterisation on exudation and mucilage release. The *highCO2* and *highMB* parameterisation, associated with high microbial C usage rates resulted in lower concentrations of dissolved low molecular weight organic C ($C_L^l$ $mol\ C/cm^{-3}$). This lower $C_L^l$ increased passive exudation. The higher exudation was then compensated by the plant starch reserves (in the mesophyll and around the plant transport tissues) and did not affect the plant growth or maintenance. As the mucilage release rate is a function of the plant starch content, higher exudation induced lower mucilage release.

These differences in exudation and mucilage release appeared only after the onset of the dry spells. The release rates between the biokinetic parameterisations for *earlyDry* became similar again from the third day after the end of the dry spell onward. The highest exudation rate per unit of root surface for a single segment was obtained at $11\ day\ 5hrs$ with *baseline* and *lateDry* ($0.153\ mmol\ C\ cm^{-2}\ d$), at $10\ day\ 21hrs$ for *highCO2* and *lowMUptake* with *earlyDry* ($0.145\ mmol\ C\ cm^{-2}\ d$), and at $12\ day\ 8hrs$ for *highMB* with *earlyDry* ($0.148\ mmol\ C\ cm^{-2}\ d$).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


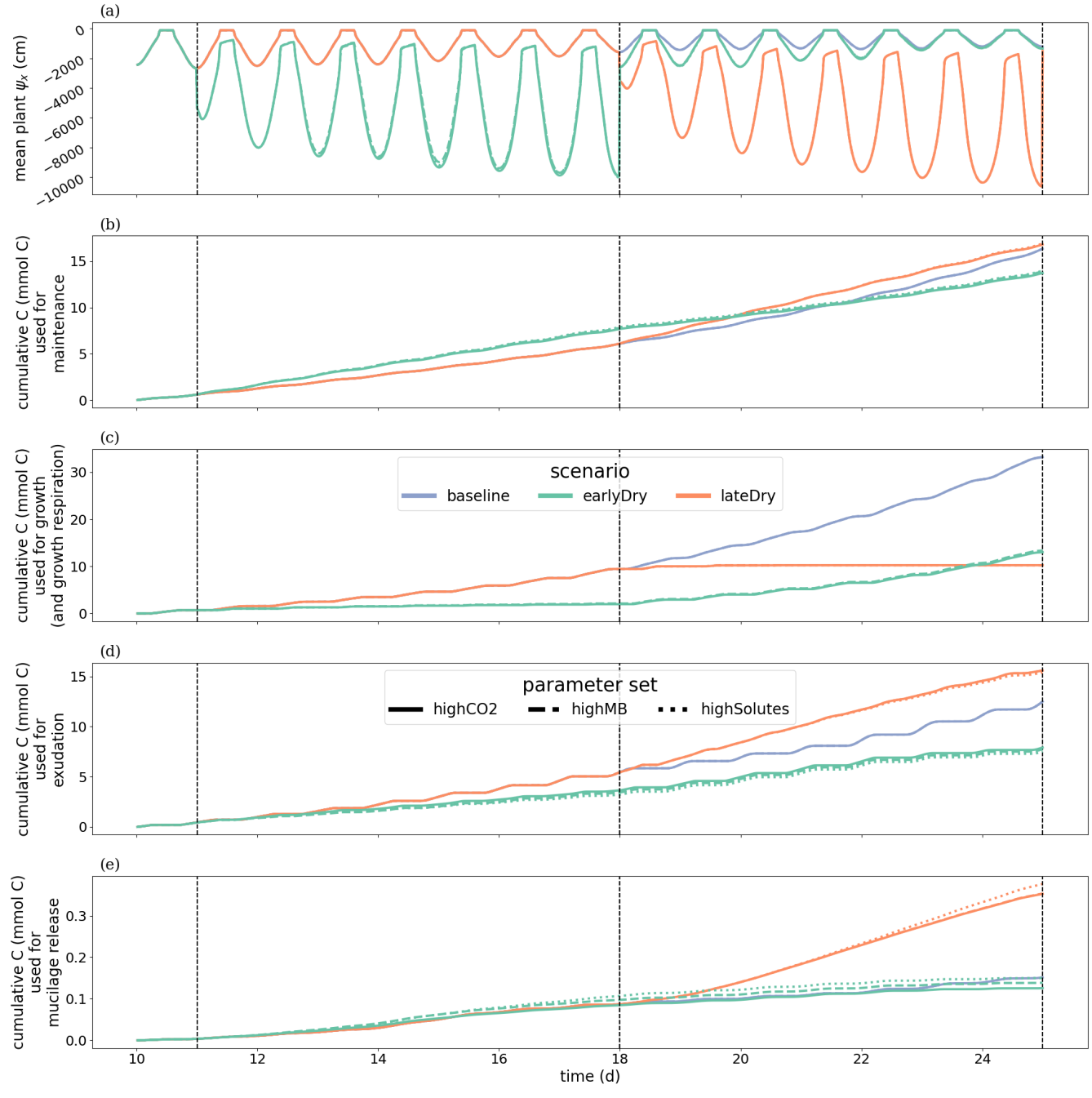


**Figure 7. Dynamics of Plant water- and carbon-related metrics:**

(**A**) the mean plant xylem water potential ($\psi$), (**B**) cumulative carbon growth and growth respiration, (**C**) exudation, (**D**) mucilage release. Line colours indicate the weather scenarios: baseline (blue) against an early (green) and late (red) dry spell. Line types represent different biokinetic parameter sets. The vertical dotted lines show the beginning and end of the early (day 11 to 18) and late (day 18 to 25) dry spells. Please note that the scales of the y-axis differ in each subplot.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 3.3 Vertical concentration profiles

Fig. 8 presents the vertical concentration profiles of organic C, microbial pools and produced $CO_2$ from microbial respiration at the end of the simulation for the bulk soil scale. The root system structure affected the concentration profiles. The peaks of organic C between $0\ cm$ and $13\ cm$ of depth corresponded with the location of the highest root length density (Fig. 8(a), (b), (c) and Fig. J1). A second peak of maximum C concentration was observed at the bottom of the profile close to the tips of primary roots. That second peak is especially strong for *lateDry* due to lower root growth, i.e., very few root segments reached $20\ cm$, such that the mean C concentration equals the maximum concentration. Conversely, the higher lateral dispersion of the roots in the upper soil layers led to a stronger lateral variability in the concentration profile (larger min-max ranges). Stronger plant growth under *baseline* resulted in perirhizal zones and rhizodeposition at lower depths such that the C accumulation at the root tips was much less pronounced compared to the dry spell scenarios.

The biokinetic parameterisation strongly influenced the C concentration profiles (Fig. 8(e)-(j)). With *highCO2*, solute and microbial C concentrations ($C_L^l, C_L^s, C_H^l, C_C, C_O$) were lowest. The *highMB* parameterisation also led to low solute concentrations but triggered increased microbial C due to higher microbial C consumption. With *lowMUptake*, solute concentrations were highest because of low microbial C uptake. These results are consistent with the observations obtained during the model conditioning (see appendix I).

Although the weather scenarios had a less pronounced effect on the concentration profiles than the biokinetic parameterisation, the dry spells induced distinct effects. Under *earlyDry*, the concentration profiles were close to that of *baseline* (e.g., $C_C$, Fig. 8(e)), or between *baseline* and *lateDry* (e.g., $C_H^l$, Fig. 8(b)). This shows the resilience soil C cycling to the early dry spell. In particular, despite the lower total exudation, the concentration of $C_L^l$ for *earlyDry* is close to that of the *baseline* due to the increased exudation rate during the second half of the simulation (Fig. 8(a)). Under *lateDry*, we observed higher $C_H^l$. This can be attributed to higher plant mucilage release for this scenario (Fig. 8(b)). The highest $C_C^a$ and $C_O^a$ values at the last time step are obtained with *baseline* (Fig. 8(g), (h)). The differences in the microbes' activation can partly be explained by the water content remaining at the high default value ($-100\ cm$) during the whole simulation under *baseline*. C uptake by copiotrophs was higher (high $C_C$, and microbially respired C as $CO_2$ but lower $C_L^l$) under *lateDry* for *highCO2* and *highMB* (Fig. 8(d), (e)). This results can be linked to the higher total exudation and lower water content, making the C ressources more readily available to the microbes. However, for *lowMUptake*, the higher C uptake by copiotrophs occurred under *baseline*. Thus, water was relatively more limiting than C supply for copiotrophic growth with *lowMUptake* (compared with *highCO2* and *highMB*) because of a lower maximum uptake rate. For that same reason, maximum $C_O$ for each parameter set is very slightly higher ($< +0.7\%$) under *baseline*.

Due to the short simulation time, $C_O$ (Fig. 8(f)) showed no significant growth at the bulk soil scale ($< 3\%$ of growth), but the dry spells weakly affected the proportion of active and dormant oligotrophs (Fig. 8(h), (j)).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


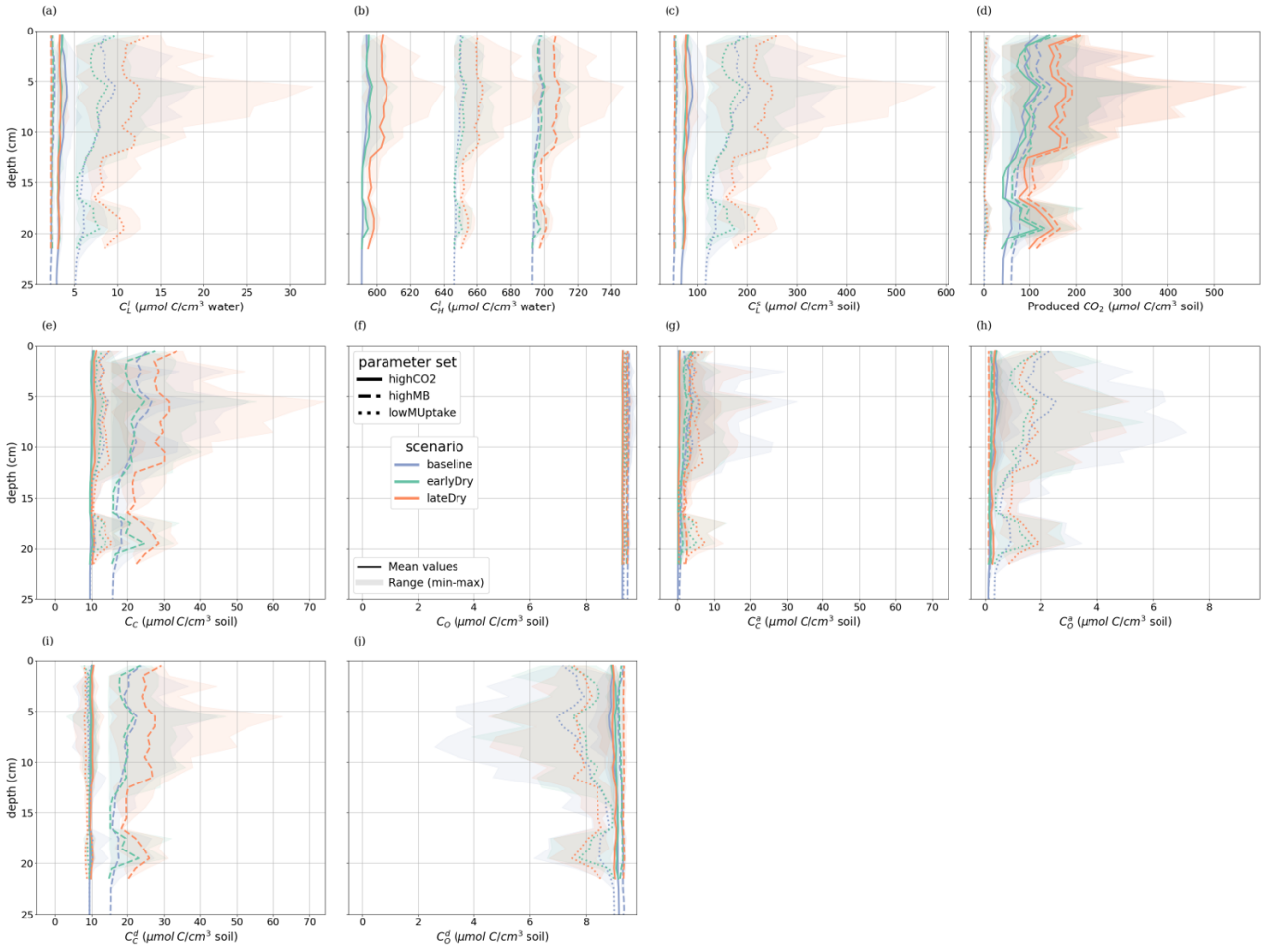


**Figure 8. Mean bulk soil concentrations of the soil carbon with depth**

(**a**) dissolved and (**c**) sorbed ($C_L^s$) low-molecular-weight organic molecules, (**b**) high-molecular-weight organic molecules($C_H^l$), (**d**) produced $CO_2$, (**e, g, i**) total ($C_C$), active ($C_C^a$) and dormant ($C_C^d$) copiotrophs, (**f, h, j**) total ($C_O$), active ($C_O^a$) and dormant ($C_O^d$) oligotrophs. Line colours indicate the weather scenarios: baseline (blue) against an early (green) and late (red) dry spell. Line types represent different biokinetic parameter sets. The semi-transparent bands give the range between the minimum and maximum concentration in soil voxels with at least one root segment at each depth.

### 3.4 Complementary cumulative volume distributions

Fig. 9 shows the perirhizal$_{trunc}$ volume with a concentration inferior or equal to the value on the x-axis. The description and motivation of the evaluation method for this figure are given in section 2.4.4. A video presenting this graphic for each time step is available in the supplementary documents ("Video S1"). Root exudation and mucilage release triggered concentration peaks of solutes and microbial C in the perirhizal$_{trunc}$ volume (Fig. 9). Particularly copiotrophs were strongly stimulated reaching high abundances up to $580\ \mu mol/cm^3\ soil$ for *lateDry* with *highMB*. Both dry spells led to strongly reduced total

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


perirhizal$_{trunc}$ volumes at the end of the simulation of $42\%$ for *earlyDry* and $34\%$ for *lateDry* in relation to *baseline*. As a consequence, maximum $C_H^l$ and $C_C^l$ concentrations were lowest with *baseline* because the released plant C triggering copiotrophic growth was distributed in a larger volume.

While *lateDry* with *highCO2* and *highMB* caused the highest $CO_2$, $C_C$ and $C_C^d$ peaks at the bulk soil scale (see respectively Fig. 8(d), (e), (i)), for the perirhizal$_{trunc}$ zone the highest values for these parameter sets were obtained with *earlyDry* (Fig. 9(c), (d), (f)). The simulated copiotroph growth during the dry spell occurred earlier under *earlyDry*, creating a larger pool of $C_C^d$ ready to be re-activated and grow during periods of high exudation. As the growth rate is a function of the current $C_C^a$, high $C_C^d$ early in the simulation favoured the overall growth in those hotspots.

Parameterizing the model with *highMB* under *lateDry* caused an especially high $C_C$ over most of the perirhizal$_{trunc}$ volume with an increase of active and a strong build-up of dormant copiotrophs (Fig. 9(d), (e), (f)). Conversely, although *highMB* under *lateDry* also led to a slight increase in the total and dormant oligotrophic concentrations (Fig. 9(g), (i)), it resulted in a decrease in the amount of active oligotrophs (Fig. 9(h)). This simulated pattern indicates a pronounced competition between oligotrophs and copiotrophs for this scenario-parameter set combination. Indeed, the $C_O^a$ values started decreasing strongly during the second half of the late dry spell, when the exudation rate became also lower.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


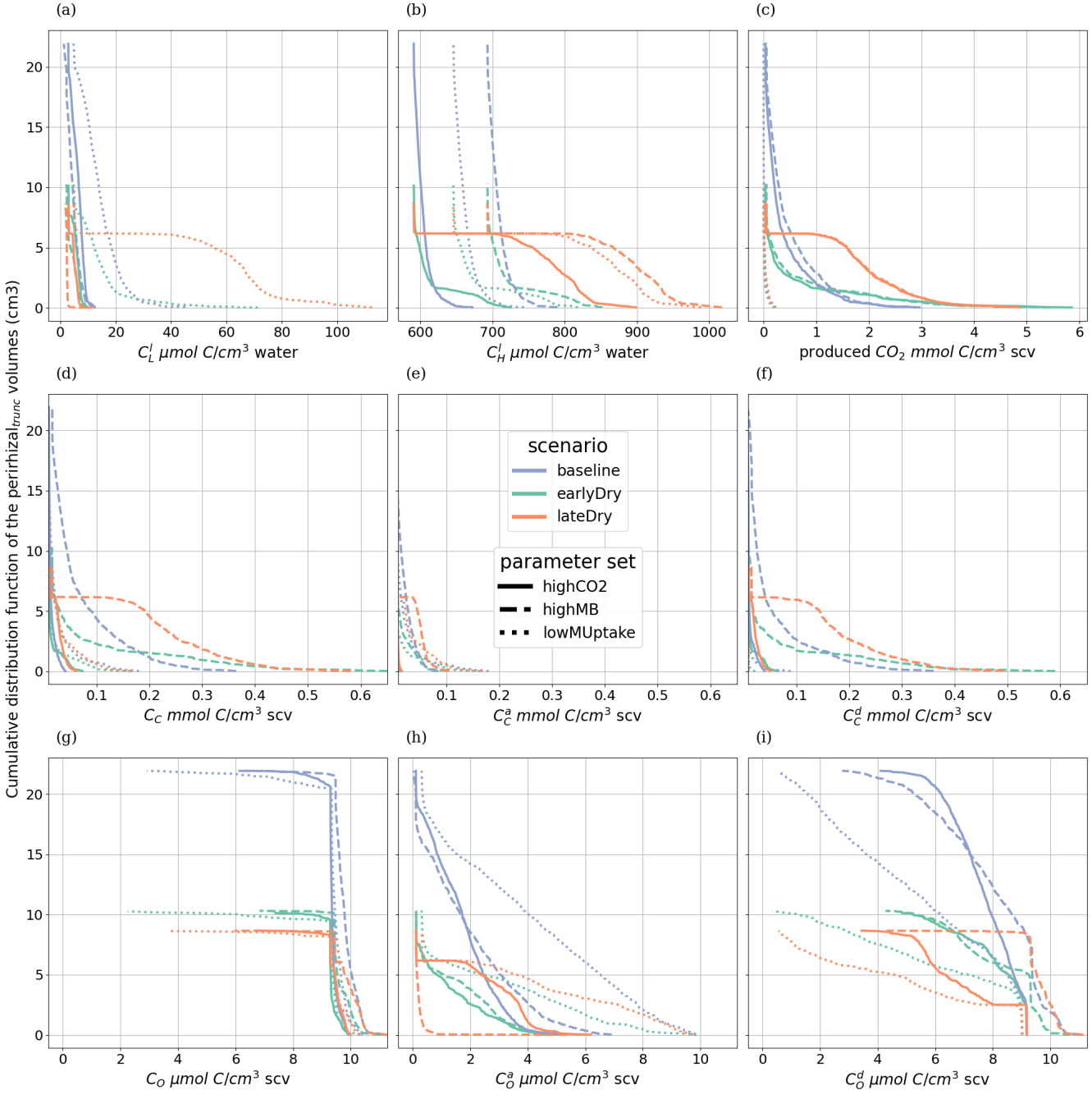


**Figure 9. Perirhizal zone volume according to the minimal concentration of organic carbon in the truncated perirhizal zones**, for (**a**) carbon of low-weight dissolved organic molecules ($C_L^l$), and (**b**) carbon of high-weight organic molecules in the water phase ($C_H^l$), (**c**) emitted $CO_2$, (**d**) total ($C_C$) (**e**) active ($C_C^a$) (**F**) dormant ($C_C^d$) copiotrophs in the soil phase, (**g**) total ($C_O$) (**h**) active ($C_O^a$) (**i**) dormant ($C_O^d$) oligotrophs in the soil phase. The line colors give the weather **scenario**: baseline (blue) against an early (green) and late (red) dry spell. The line types represent the different biokinetic parameterisation. Subplots d, e, f and g, h, i have the same scale on the x-axis.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 3.5 Carbon pool distribution

We wished to evaluate the changes in C turnover within the plant-soil system, according to the weather scenarios and for the different biokinetic parameter sets. Consequently, Fig. 10 gives the relative changes of C content in different C pools, compared with the *baseline* scenarios. The relative increases of activated microbes-C and solutes-C (Figs. 10.B and 10(c)) correspond to the night periods, when less C was exudated with *baseline* compared with the other scenarios. These periods also corresponded to higher soil matric potentials, diminishing the negative effects of the low soil $\theta$ on microbial activation during the dry spells. This relatively higher activated microbes-C pool was observed for the *highMB* and *highCO2* parameter sets with *lateDry*, although the values were lower than for *baseline* at the last time step. The *lateDry* scenario led consequently to a redistribution of C in the microbial and emitted $CO_2$ pools. Therefore, in spite of the higher total exudation, the solutes-C pool is lower compared with the corresponding *baseline* scenarios. On the contrary, for *lowMUptake*, the *lateDry* scenario led to a higher accumulation of C within the solutes pools (Fig. 10(d)). We can also note that, while we have converging relative solutes-C values between *earlyDry* and *lateDry* for *highMB* and *highCO2* by the end of the simulations, the values for *lowMUptake* are diverging. For all *earlyDry* scenarios, we observe that less C enters the soil domain, leading to relatively lower values compared with *baseline* for all pools by the end of the simulations. We also found a small relative uptick of activated microbes-C for the *highMB* and *highCO2* parameter sets after the spell (Fig. 10(b)), linked with the increased soil water content and plant exudation (Fig. 7).

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Preprint. Discussion started: 7 March 2025


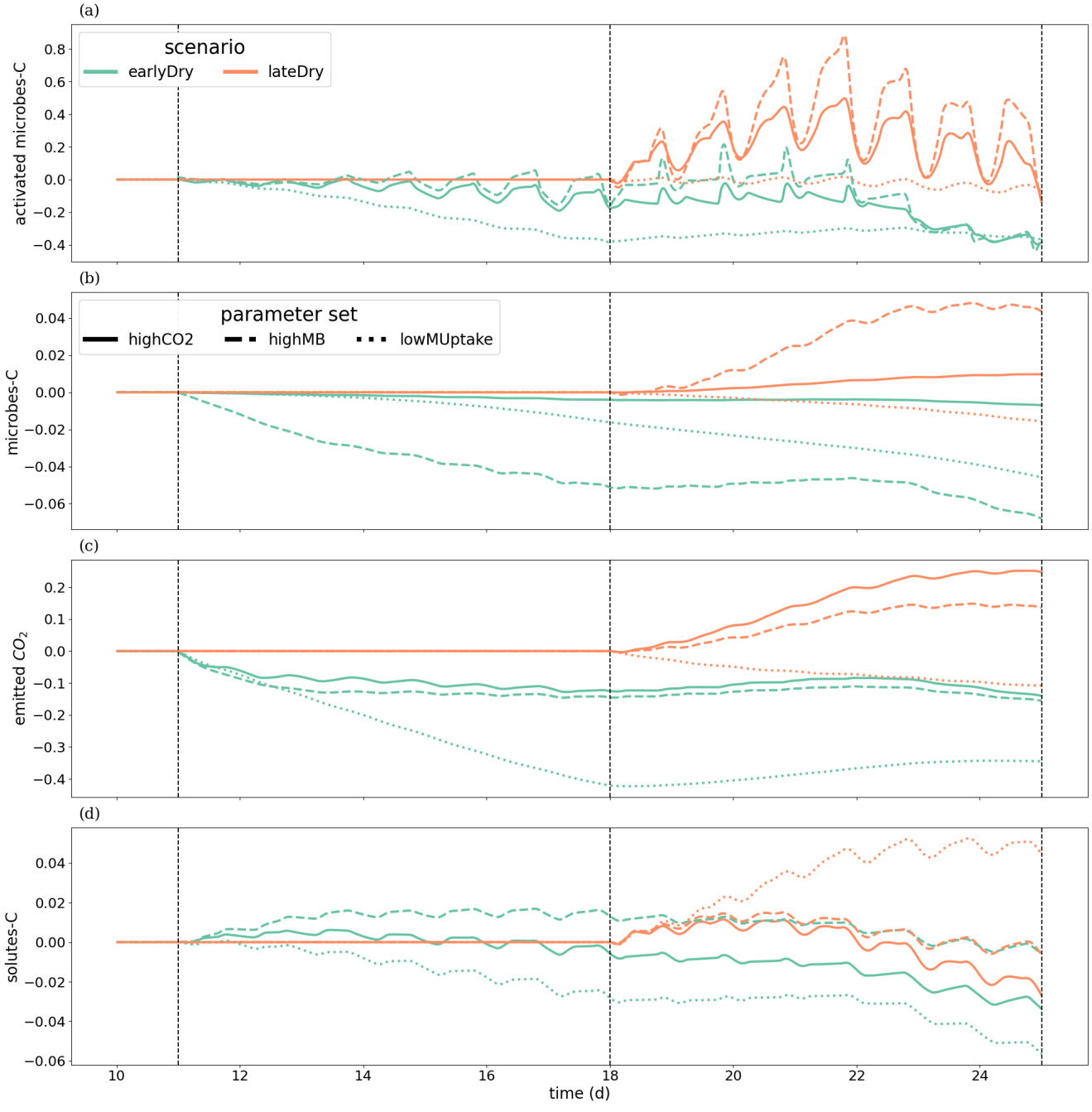


**Figure 10. Relative change of root-released carbon use in response to drought scenarios according to the biokinetic parameters at the macroscale.**

The panels present the difference of C between each drought treatment and the baseline in relation to the baseline C usage for (a) microbes-C, (b) activated microbes-C, (c) $CO_2$ emitted by microbes, (d) soil solutes-C. The line types represent the different biokinetic parameterisation. The dotted lines show the beginning and end of the early (day 11 to 18) and late (day 18 to 25) dry spells. Please note that the scales of the y-axis differ in each subplot.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 3.6 SOC hotspots

To evaluate the root systems' exudation efficiency, Fig. 11 presents the relative volumes of the SOC hotspots (see definition in 2.4.5) in the bulk soil. We observed distinct characteristics over the whole simulation for each biokinetic parameterisation. For *highCO2*, the absolute hotspot volume remained low and decreased with growth (after an initial increase during the dry spells). For *highMB*, the total absolute hotspot volume ($SOC \geq 0.65 SOC_{expected}$) peaked in the first half of the simulation before becoming stable under *baseline*. With this biokinetic parametrisation, we observed the portion the relative hotspot volume within the highest class ($SOC \geq 1.16 SOC_{expected}$): $8\%$, $32\%$, and $29\%$ of the hostpot volume belonged to the highest class under, respectively, *baseline*, *earlyDry*, and *lateDry*. Because of the low microbial activity, we observed the highest relative SOC hotspot volume for *lowMUptake* for all weather scenario: $2.9e-2$, $2.8e-2$, and $0.11$ under *baseline*,*earlyDry*, and *lateDry*.

Outside of the dry spell, diurnal cylcing in the hotspot volume followed the plant C releases during the day and soil C mineralisation without replenishment at night. This dynamic is especially strong with *highCO2* as the hotspot volume is (almost) back to $0$ at the end of the day periods. The dry spells buffered the diurnal cycle for all scenarios as the exudation became more stable. Moreover, the biggest hotspot volume and intensity were obtained with the *lateDry* spell, following the higher exudation and mucilage release. *earlyDry* did not lead to a higher total hotspot volume (with $SOC \geq 0.65 SOC_{expected}$) for the *highMB* and *lowMUptake* parametrisation at day 25 of growth. However, a bigger portion of the SOC hotspost belonged to the higher hotspot classes ($\geq 0.83 SOC_{expected}$ or $\geq 1.16 SOC_{expected}$).

For *highCO2* and *highMB*, we observed an increase in hotspot volume during the first half of the dry spells, followed by a decrease during the second half. This can be partly explained by the decrease in daily plant C releases during the second half of the spell. The decreasing SOC hotspot volume in the second half of the spells was also due to the activation and growth of the microbial communities and C utilization after the first strong influx of plant C releases, followed by partial dormancy. Upon the next influx of C (the following day), the microbes reactivated and used the C more quickly. For *lowMUptake*, characterised by its lower microbial activity, we observed a continuous increase in hotspot volume throughout the spells.

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Preprint. Discussion started: 7 March 2025


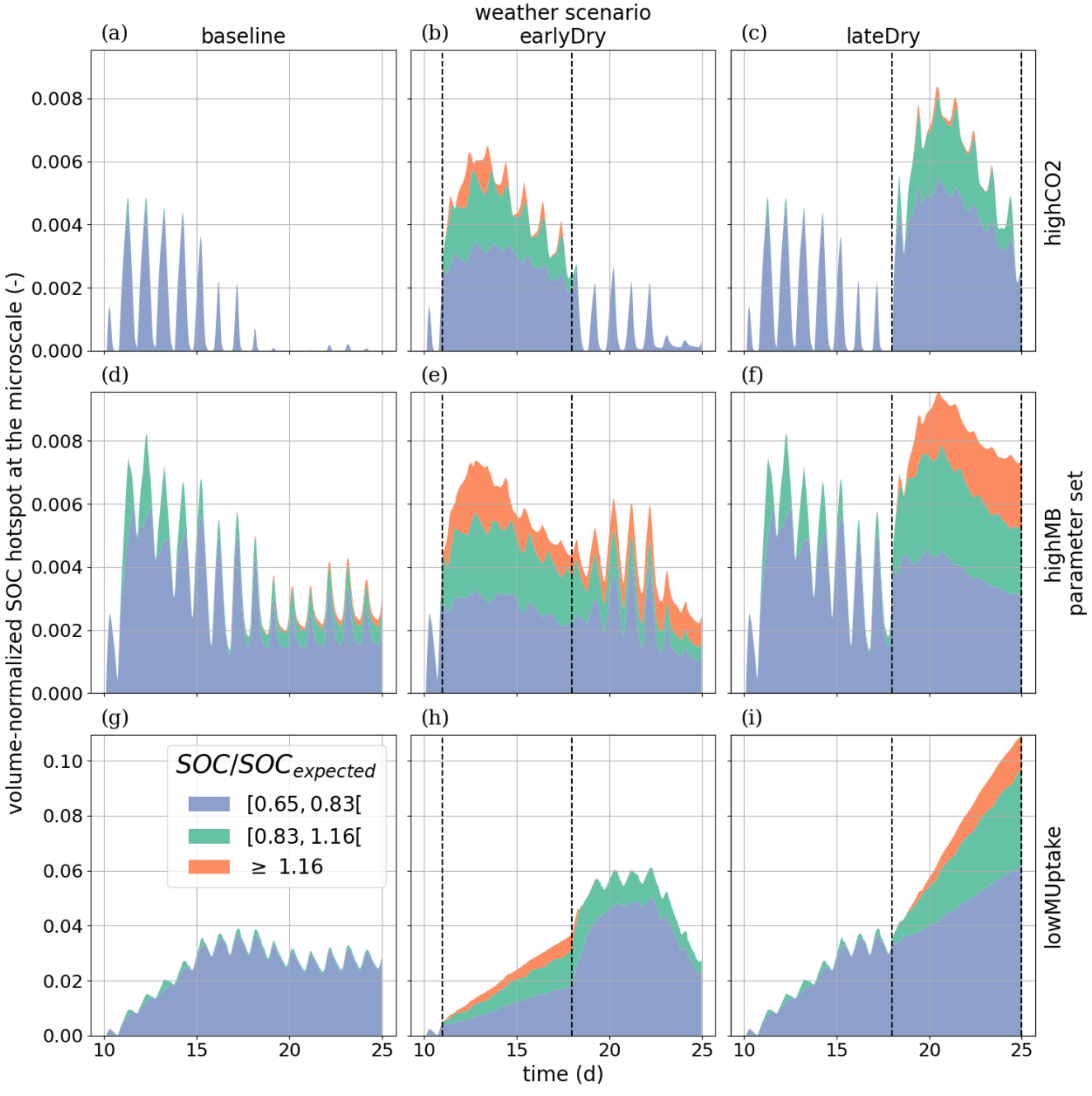


**Figure 11. Relative SOC hotspot volume in the perirhizal zone according to time** for the three $SOC/SOC_{expected}$ classes. The classes' ranges were defined according to Poeplau and Don (2023). The dotted lines show the beginning and end of the early (day 11 to 18) and late (day 18 to 25) dry spells. The third row is on a scale different from the first and second rows.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 3.7 Radial carbon concentration profiles

To analyse how plant-soil system responses to drought affect the carbon stabilisation in the perirhizal zone, Fig. 12 shows the connection between the extent of the microscale domains and dissolved low-weight organic molecules concentrations $C_L^l$ at the end of the simulation. Just as for the bulk soil and perirhizal$_{trunc}$ scales, the highest $C_L^l$ were obtained under *lateDry* for *lowMUptake* and under *baseline* for *highCO2* and *highMB* (see Fig. K1). For *lowMUptake*, microscale domains with shorter outer radii (segment index eight, which is nearer to the root surface) had higher radial concentrations. These shorter outer radii were caused by several microscale domains sharing a single macroscale voxel. Therefore, the higher concentrations underline the additive effect on the $C_L^l$ profile due to proximity to the perirhizal zone, which can indicate an overlap of the rhizospheres. This proximity effect was less noticeable for *highCO2* and *highMB*, where we observed concentration profiles less dependent on the extent of the microscale domain. Indeed, with those biokinetic parameter sets, the microbial C uptake was highest and reacted fastest to high influxes of dissolved low molecular weight organic carbon. Therefore, the $C_L^l$ was closer to an asymptote at the outer boundaries of the 1D domain. These steeper gradients can cause a the rhizosphere extent to be smaller, limiting the rhizosphere overlaps. The effect of rapid microbial C uptake with *highMB* is also visible in Fig. 12(d) and E, where some concentration profiles show lower $C_L^l$ values closer to the root surface, where the concentration of $C_C$ is highest (see Fig. K). The $C_L^l$ radial profiles are strongly linked to the $C_C$ profiles, as presented in appendix K.

The supplementary video "Video S2" shows $C_L^l$ and the corresponding $C_C^a/C_C$ ratios at each time step. We found a high microbial growth during the first pulse of added C followed by a transition to dormancy due to reduced C availability. Microbes remained mostly dormant until reactivated by the next C input pulse while also slowly dying. Reactivation of the microbes during the periods of high $C_L^l$ led to a rapid consumption of the carbon in dissolved low-weight organic molecules near the root surface. As a result, $C_L^L$ became lower than it initially was once the C input pulse diminished–at night (e.g., day 24.69 of growth) and during the second half of the dry spells. We can also observe how, during the dry spells, $C_L^L$ were higher than for the other two scenarios due to lower water content, favouring microbial C uptake.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


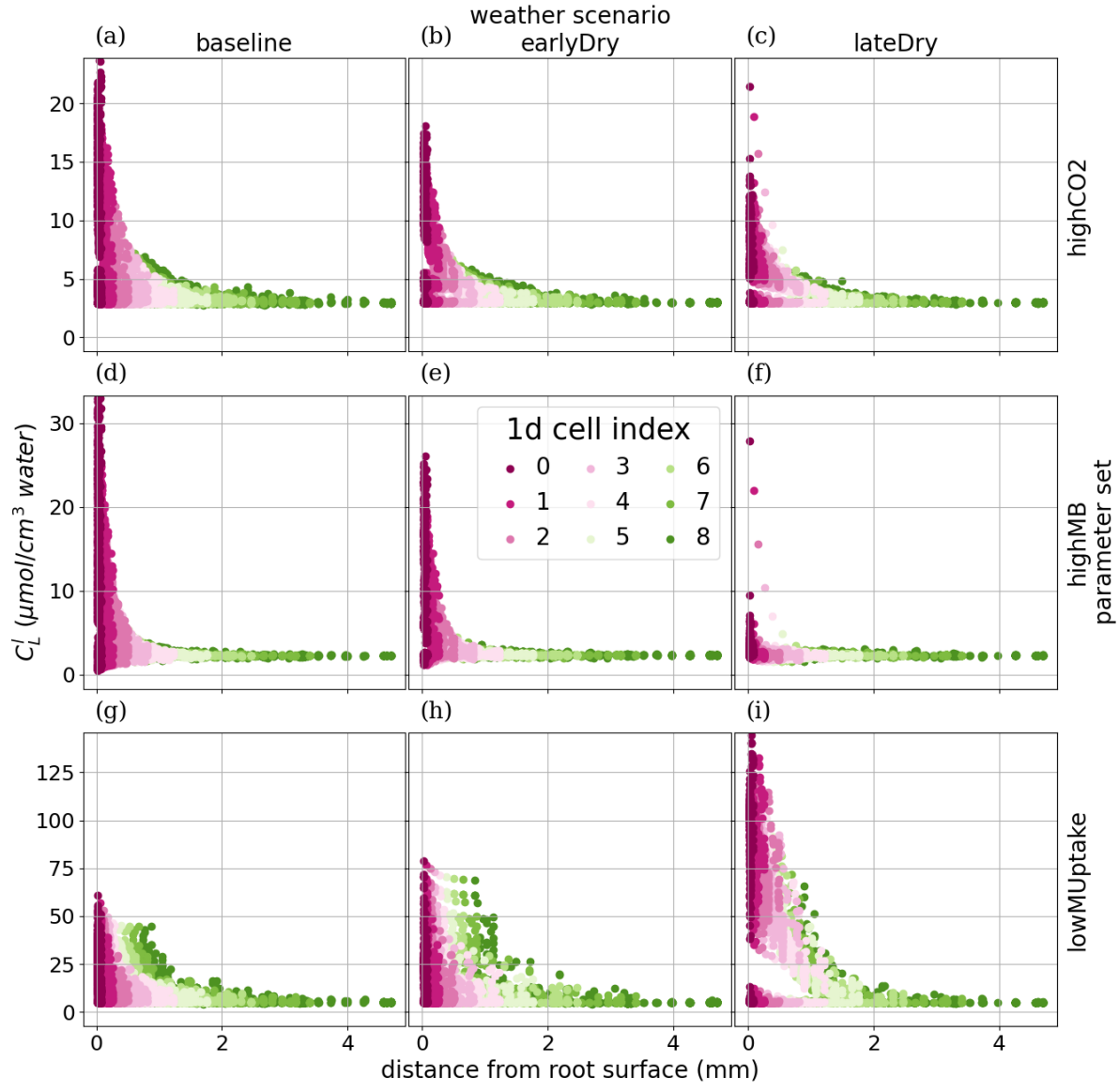


**Figure 12. radial concentration profile of carbon from low molecular weight organic compounds** at the end of the simulation for each plant perirhizal zone. $r$ $(mm)$ corresponds to the distance to the root surface. The colour gives the segment index of the 1D domain. Each column corresponds to a specific weather scenario and each row corresponds to a specific biokinetic parameterisation.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


# 4 Discussion

## 4.1 Model setup

Several models have been developed to simulate the root-influenced spatiotemporal distribution of carbon (C) turnover and microbial activity (Pot et al., 2022; Sırcan et al., 2025), the exudation from a growing 3D root system (Rees et al., 2023), or the exudation and water uptake by a static plant, based on the C and water balance within the plant and soil (Lacointe and Minchin, 2019; Zhou et al., 2020). Rees et al. (2020) coupled *RhizoDep* with other models on the *OpenAlea* platform to represent the root-soil C and nitrogen exchanges for a growing wheat plant, driven by its inner nitrogen and C balances. Regarding plant-soil coupling for solute flow using FSPMs, several modelling studies have represented the soil as a dynamic environment with water and solute uptake (generally phosphorus) or $C$ releases from a static or growing root system (Ruiz et al., 2021; Schröder et al., 2014; Jorda Guerra et al., 2021; Gérard et al., 2017; Mai et al., 2019; Heppell et al., 2016; Landl et al., 2021a; Schwartz et al., 2016). Braghiere et al. (2020) set up a 3D FSPM accounting for shoot-root-soil interactions for water and C using model coupling. However, their framework did not account for either C flow and microbial reactions in the soil or inner plant water and C balance. Some coupled models also represented inner plant water flow (Schröder et al., 2014; Mai et al., 2019; Schwartz et al., 2016), or root-shoot interactions (Heppell et al., 2016; Braghiere et al., 2020), and Mai et al. (2019) used a sequential implementation of the multi-scale setup. Our framework stands out by coupling of a dynamic whole plant model with a dynamic soil model for both water and C flows (Ruiz et al., 2021; Rees et al., 2018; Schnepf et al., 2022), including biochemical and physical reactions (such as adsorption and the interactions with microbial communities) in the soil domain. The multi-scale framework is a further advantage of this fully open-source setup (Ruiz et al., 2021), increasing the resolution in the soil areas near the root-soil interface to balance accuracy and computing speed. Moreover, the use of fixed-point iteration with implicit time stepping allowed for larger time steps, increasing therefore not only the model accuracy but also its speed for specific scenarios. However, as the simulation of the water flow was the main bottleneck for model convergence, application of the model to more sandy soil will lead to shorter time steps and, therefore, longer computation time. There remains potential for further optimization the code in order to increase its computing speed.Expending the framework presented by Schnepf et al. (2018b), this coupled model remains flexible, allowing the user to implement only the modules relevant to their research question. The high number of functions represented lead to a high number of parameters. However, several structural plant or root system parameter sets have been established for different species. Moreover analysis of the structural root system module were conducted by Schnepf et al. (2018a) and Morandage et al. (2022). For the soil biokinetics, Sırcan et al. (2025) defined a parameter space that fulfills biogeochemical constraints identified from a literature study. They also conducted a sensitivity analysis of the outputs. A user-friendly implementation of the CPlantBox calibration method of Morandage et al. (2021) is currently being developed. Finally, this implementation of TraiRhizo in DuMu$^x$ within CPlantBox sets the building blocks for the simulation of new processes, taking into account solutes such as phosphorus and nitrogen, and the biological, chemical or physical reactions they are subject to.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### 4.2 Plant processes

In this implementation of the model, we simulated a simplified plant C dynamic compared with the one described in the literature, while still being able to re-create qualitative plant dynamic. Simulation results indicate that plant expansion growth is strongly influenced by changes in water potential during the diurnal cycle and drought periods, consistent with processes described in previous studies (Verbančič et al., 2018; Barillot et al., 2020; Coussement et al., 2018; De Swaef et al., 2022). However, it is hypothesised that cell wall biosynthesis (biosynthetic growth) predominantly occurs during the day using photoassimilates, while being much more limited at night when it relies on starch reserves (Verbančič et al., 2018). Although our simulations did not explicitly separate biosynthetic growth from expansion growth, the parametrization of the plant C module allowed us to qualitatively reproduce these dynamics. For this simulation, the virtual plant's starch pool can be interpreted as representing both actual starch reserves and newly synthesised wall material, thereby enabling expansion growth to occur at night. To achieve robust results and better recreate typical C dynamics across a wider range of parameter sets, it could be beneficial to explicitly represent biosynthetic growth in future models. Following the analyses of Verbančič et al. (2018) and Barillot et al. (2020), high biosynthetic growth requires higher C supply but results in the creation of new cells more flexible and capable of expanding under lower turgor pressure. This higher amount of cells with high cell wall flexibility can help maintain plant growth in case of drought (Blum, 2017). Another mechanism supporting growth under low turgor pressure is osmotic adjustment, which has been identified as a critical process during drought conditions (Blum, 2017; Coussement et al., 2018). Not including this process in our model could explain the high growth limitation caused by drought observed in our simulation.

Regarding the plant's C release, exudation was found to be positively correlated with plant growth (Přikryl and Vančura, 1980; Canarini et al., 2019). In our study, we assumed that exudation occurs only at the growing root tip, making the two correlated on the diurnal- and weekly-scales for a specific weather scenario. However, lower growth allowed more $C$ to be available for exudation, making the two anti-correlated on the hourly scale (day vs. night dynamics) and when comparing dryer against wetter scenarios. Moreover, in experimental studies, a decrease of rhizodeposits was also observed at night (Kuzyakov and Cheng, 2004). This dynamic was particularly strong in our simulations, as we observed no exudation in the middle of the night outside of the dry spell periods. However, we could still recreate qualitative observations made in other studies. Indeed, plants to regulate internal C concentrations and adjust C allocation for growth and maintenance under fluctuating environmental conditions by modulating starch storage (Tixier et al., 2023; Bazot et al., 2005) and C release rates (Prescott et al., 2020; Canarini et al., 2019). The upper range of our exudation rates per unit of root surface ($\approx 0.16\ mmol\ C\ cm^{-2}\ d$) was superior to the averaged rates given in the experimental study of Kravchenko et al. (2004) ($0.018\ mmol\ C\ cm^{-2}\ d$) or Trofymow et al. (1987) ($0.01\ mmol\ C\ cm^{-2}\ d$, as presented by Darrah (1991)). However, we could find similar values in the study of Personeni et al. (2007, Fig3A), due in part to its higher temporal resolution: $\approx 0.68\ mmol\ C\ cm^{-2}\ d$ under high light input and assuming an exuding root tip of $1\ cm$. The modelling study of Thorpe et al. (2011) for a dwarf bean plant yielded $\approx 0.69\ mmol\ C\ cm^{-2}\ d$, assuming and exuding root tip of $1\ cm$ with radius of $0.02\ cm$. Moreover, microbial C uptake acted as a C sink and could affect the exudation rate (Canarini et al., 2019). We also observed a change in the type of organic $C$

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


released by the plant (in our model, exudation-to-mucilage release ratio) under dry spell (Bazot et al., 2005; Hartmann et al., 2020). In spite of those changes, mucilage remained between 1-10% of exudation, consistent with the observations of Nguyen (2009), and exudation represented between 3-40% of assimilated C (Dilkes et al., 2004; Lynch and Whipps, 1990).

Regarding the plant water balance, the outputs of the model differ from that presented by Giraud et al. (2023), in part because of the implementation of the multiscale setup with fixed-point iteration, in part because of the update of the plant parameters, as decribed in section 2.3.

### 4.3 Distribution of soil carbon

#### 4.3.1 Spatial and temporal distribution of microbial functional groups

Regarding the spatial resolution, we observed a smooth gradient of low-weight dissolved organic molecules-C ($C_L^l$) along the radial axis for the different biokinetic parametrisation. This suggests that our resolution for the microscale domains is sufficient to represent the C flow in the 1D soil models. For simulations of solutes with low diffusion rates (e.g. phosphorus) and a lower advection (low plant water uptake rate), the root's uptake rate would become strongly dependent on the size of the 1D segment at the root-soil interface. A study could be conducted to evaluate the minimum number of segments necessary to accurately represent the selected soil processes according to the range of expected advection and diffusion rates of solutes under specific scenarios. The output of the simulations showed diverging results according to the studied scales (macroscale, bulk soil, perirhizal$_{trunc}$ and microscale). For instance, compared with the bulk soil scale, the perirhizal$_{trunc}$ scale showed a higher influence of the weather scenarios on the soil C balance. Moreover, the microscale showed a high gradient of the C concentration along the radial coordinate of the 1D domains that could not be represented via the perirhizal$_{trunc}$ scale. These scale-dependent results underline the advantage of using a multi-scale simulation and having a higher precision at the root-soil interface, following the observations of Mai et al. (2019). Moreover, the model showed a strong horizontal and vertical variability in the concentrations, making a 3D evaluation relevant before, for instance, aggregating the results to a 2D or 1D sink term to be used by higher-scales models. As mentioned in the first implementation of the multiscale framework (Mai et al., 2019), the low resolution near the root soil interface (at the $mm$ scale) raises the issue of including lower-scale processes, such as the influence of pore size on the water and C balance (Kuppe et al., 2022). As in the study of Landl et al. (2021a), the interactions between the 1D and 3D soil models also allowed us to represent the additive effect of perirhizal zone proximity, which led to higher solute concentration under specific biokinetic parameterisation (*lowMUptake*) and favored C hotspot formation from plant releases. Landl et al. (2021a) also evaluated the influence of root traits on the soil's normalised hotspot volume. Our study complements those findings and shows that root and microbial traits have to be evaluated together, as high concentration of soil organic C can be reached for different exudation rates according to the traits of the microbial community.

Other characteristics of the microbial activity were studied with our model. With the biokinetic parameter sets *highCO2* and *highMB*, we observed a diurnal dynamic of high microbial growth under higher exudation (daytime), leading to a high

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


consumption of C for microbial growth and maintenance. This was followed by microbial dormancy (high dormant-to-total microbe ratio at nighttime). This dynamic has been observed in the literature and can be described as a "starving-survival lifestyle", where microbes enter dormancy in a low-nutrient environment and quickly react to new inputs of resources (Hobbie and Hobbie, 2013). We found a specific reaction to resource scarcity for the parameter set *highMB* with $lateDry$. For this simulation, we found an especially high copiotroph growth and a high ratio of dormant oligotrophs. This diverging results between the two communities are indicative of a possible intra-microbial competition. This follows over studies where plant exudation and root growth affected microbial composition (de la Fuente Cantó et al., 2020; Bonkowski et al., 2021). Biokinetic parameter sets describing more active microbes (*highCO2* and *highMB*) were also linked to a higher usage of soil solutes in case of higher exudation, when compared with the *baseline* scenarios. This higher usage rate led to a form of "rhizosphere priming effect" (Bonkowski et al., 2021; Kuzyakov and Cheng, 2004) where the root exudation caused an increase in mineralisation of the pre-existing soil organic matter, leading ultimately to a relatively lower amount of C in the solute pool compaired with the *baseline*. A more precise evaluation of a possible rhizosphere priming effect could be conducted with this setup, by dividing each C pool between the C originating from the plant additions and the C already present in the system at the beginning of the simulation. Our simulation of the microbial dynamic and competition was however limited by not accounting for other stresses than C and water scarcity, such as nitrogen, phosphorus (Drake et al., 2013; Brown et al., 2022), or oxygen (Wiesenbauer et al., 2024) scarcity. Likewise, the diurnal aspect of microbial activity would also be better represented by accounting for soil temperature (Kuzyakov and Cheng, 2004). However, over the time period of this study (two weeks), we assumed the soil temperature varied little. Regarding the spatial distribution of the microbes, the prescribed exudation near the plant root tips also led to a higher microbial growth in those areas, resulting in a vertical distribution similar to the one observed by McDougall and Rovira (1970). At the microscale, simulations also resulted in very high concentrations of copiotrophs near the root surface. Although high copiotrophic concentration near the root surface following exudation is expected (Bonkowski et al., 2021), representing microbial motility (Kuppe et al., 2022; Schnepf et al., 2022) would help smooth these concentration peaks. Representing motility could also potentially lead to a better representation of the priming effect as the microbes (especially from mature roots) might diffuse and consume C in areas further away from the root-soil interface (Dupuy and Silk, 2016).

#### 4.3.2 Effect of dry spells on carbon stabilisation

The biokinetic parameterisation strongly influenced the effects of the weather scenarios on soil C balance. For more active biokinetic parameter sets (*highCO2* and *highMB*), the microbial growth was limited by C resources. The higher plant C releases *lateDry* had therefore a positive effect on the microbial community. On the contrary, for non-C limited microbial communities (*lowMUptake* parameter set), the water stress of *lateDry* affected negatively the microbial growth. These opposite reactions influenced how the soil domain was impacted by the short dry spells (see below). The microbial dynamic will have an even stronger impact on the simulated water and C balance once soil-to-plant feedback mechanisms are implemented, such as nutrient uptake (de la Fuente Cantó et al., 2020) and organic C-dependent soil hydraulic parameters (Landl et al., 2021b; de la Fuente Cantó et al., 2020).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


Our $earlyDry$ and $lateDry$ weather scenarios led to a short decrease in soil water content, creating a wetting-drying cycle. According to the meta-analysis of Borken and Matzner (2009), these wetting drying cycles should lead, under specific environmental conditions and microbial communities, to lower microbial respiration during the spells, followed by a respiration pulse once the soil is rewetted. These pulses may or may not compensate for the earlier $CO_2$ emission decrease (Borken and Matzner, 2009). In our simulation, the early dry spell always led to a decrease in overall emitted microbial $CO_2$ at the macroscale when compared with the *baseline* scenarios. We then observed in the week following the end of the spell a slight uptick in emitted $CO_2$ compared with the baseline, which did not compensate the lower earlier emissions. For the later dry spells with *highCO2* and *highMB* parametrisation, the emission pulses occurred during the spells. Indeed, while the drying led to a lower portion of microbes being dormant, the soil water content often remained too high to cause high microbial death or deactivation, especially for soil zones further away from the roots (macroscale). The lower water stress was, therefore, partly compensated by the higher $C_L^l$. We did not simulate an increase of plant and microbial necromass to be used by the soil microbes at the end of the spell (increasing thus the respiration once the soil is rewetted). Another explanation for the divergence is that we do not represent the easier access to "previously protected organic matter" caused by sudden soil rewetting. Moreover, we represented short dry spells (seven days) while longer spells (two weeks) may be necessary to see stronger effects on the microbial community (Borken and Matzner, 2009). The higher C mineralisation during the drying phase of the later dry spell could also be linked to the method used to represent microbial sensitivity to water stress. Indeed, for simplicity, we did not represent the direct effect of soil water content on the potential microbial death ($k_{max}$). Moreover, we used the same value to calibrate the sensitivity of copiotrophs and oligotrophs to water stress, although oligotrophs could be assumed to be more resistant to low soil water content. Finally, the water scarcity parameters could be recalibrated using experimental data.

We could reproduce qualitatively processes measured by Deng et al. (2021) for the C balance under limited water resources. Indeed, we observed a decrease in root biomass during the dry spells, with, under some scenarios, an increased exudation. The lower root growth then led to lower plant respiration, while the higher concentration of dissolved organic C under the late dry spell (with *highCO2* and *highMB*) led to a higher microbial respiration by the end of the simulation. Contrary to Deng et al. (2021), we did not observe a decrease in total soil organic C. They linked this decrease to a lower soil C addition from plant residue, which is not represented in our model. Under $earlyDry$, we could observe (limited) differences in concentration compared with the $baseline$ seven days after the end of the dry spells, underlining the resilience of the simulated environment, especially for the soil zones nearer the roots. The $lateDry$ scenario led to the lowest plant growth but to a higher $SOC$ hotspot volume, indicating a more resource-efficient root system exudation. We had, therefore, a trade-off in the C usage strategy.

## 5 Conclusions

In this paper, we presented the equations and implementation of a coupled model representing the carbon (C) and water flow in the soil-rhizosphere-plant continuum, influenced by the atmospheric conditions via plant transpiration and photosynthesis. This new framework takes into account the effect of the water content variation on the C flow and microbial reactions. Moreover, the multiscale implementation allowed us to evaluate more precisely the water and C flow and reactions at the

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


soil-plant interface, quantifying the feedback effect of the plant on the soil processes. Thanks to the outputs of the model, we could observe the evolution of variables difficult to measure experimentally at the rhizosphere scale with non-destructive measurements, such as exudation and soil respiration. In our simulation, the effect of dry spells on the soil C balance depended on the time dynamic of the exudation and the characteristics of the microbial community, underlying the site-specific aspect of agricultural practices' effects on the C balance. For instance, compared with the baseline scenarios, dry spells could lead to an increase of C mineralisation with active microbial communities (C-limited) against lower mineralisation for less active microbial communities (water-limited). Adding nutrient (such as nitrogen) flows in the coupled model would be an important extension to represent more accurately the feedback effect of the soil C balance on the plants' development.

## 6 Code availability

. For this study, we used the plant model CPlantBox (Schnepf et al., 2025b) and the corresponding soil module (Schnepf et al., 2025a). The full setup is available at: Giraud2025_CarbonStabilisation

## 7 Video supplement

. A video presenting this graphic for each time step is available in the supplementary documents ("Video S1"). The supplementary video "Video S2" shows $C_L^l$ and the corresponding $C_C^a/C_C$ ratios at each time step.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


## Appendix A: List of the parameters and variables

**Table A1.** Represented carbon pools

| **Output variables** | Definition | Unit |
|---|---|---|
| $C_L^l/C_L^s$ | Concentration of carbon from compounds with low molecular weight (in the liquid/solid phase) | $mol\ C\ cm^{-3}\ water$ / $mol\ C\ cm^{-3}\ scv$ |
| $C_H^l$ | Concentration of carbon from compounds with high molecular weight | $mol\ C\ cm^{-3}\ water$ |
| $C_O$ ($C_O^a$, $C_O^d$) | Concentration of oligotrophs (active, dormant) | $mol\ C\ cm^{-3}\ scv$ |
| $C_C$ ($C_C^a$, $C_C^d$) | Concentration of copiotrophs (active, dormant) | $mol\ C\ cm^{-3}\ scv$ |
| $CO_2$ | Unit of emitted $CO_2$ per volume of soil | $mol\ C\ cm^{-3}\ scv$ |

## Appendix B: Soil water flow

In the sections below, we present the implementation of the equations given in section 2.2.2 to the 1D axisymmetric and 3D soil domains.

### B1 3D soil model

For the 3D macroscale soil model, the sink term of Eq. (6) $S_\theta = S_{w,root-3DS}$ ($cm^3\ water\ cm^{-3}\ scv\ d^{-1}$), the water uptake or release by the roots:

$$S_{w,root-3DS,init} = \frac{1}{V_{3DS,scv}} \sum_{i=1}^{nr} \frac{\partial \theta_i V_{1DS,scv,i}}{\partial t} \tag{B1}$$

$$S_{w,root-3DS} = \mathbf{Lim}(S_{w,root-3DS,init}) \tag{B2}$$

where $nr$ $(-)$ is the number of root segments in the soil control space of volume $V_{3DS,scv}$ ($cm^3\ scv$), the $i$ subscript is the identification of the $i^{th}$ root, $V_{1DS,scv,i}$ ($cm^3\ scv$) is the volume of the perirhizal zone $i$ and $\theta_i$ its water content. Instead of using $q_{w,root-soil}$ (see Eq. (3)) like Mai et al. (2019), in this study $S_{w,root-3DS}$ is obtained from $\frac{\partial \theta_i V_{1DS,scv,i}}{\partial t}$. This helps avoid computation errors when simulating the macro-soil flows and diminishes the divergence between the macro- and microscale models. Indeed, the plant-prescribed $q_{w,root-soil}$ was already potentially limited during the computation of

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


**Table A2.** TraiRhizo input parameters. When the source is not given, the parameter values are taken from the sets defined by Sırcan et al. (2025) and selected in section I. HMW: high molecular weight organic carbon compound.

| **Symbol** | Definition (and source) | Value per selected parameter set | | | Unit |
|---|---|---|---|---|---|
| | | *highCO2* | *highMB* | *lowMUptake* | |
| $a$ | Sharpness parameter for the switch function from active to dormancy | 0.1 | | | – |
| $C^l_{H,init}$ | Initial concentration of high molecular weight organic carbon concentration | $5.94e^{-4}$ | $6.94e^{-4}$ | $6.47e^{-4}$ | $mol\ C\ cm^{-3}\ water$ |
| $C^l_{L,init}$ | Initial dissolved low molecular weight organic carbon | $4.71e^{-6}$ | $5.15e^{-6}$ | $5.1e^{-6}$ | $mol\ C\ cm^{-3}\ water$ |
| $C^s_{L,max}$ | Maximum sorption capacity | $8.9e^{-4}$ | | | $mol\ C\ cm^{-3}\ scv$ |
| $C_{thres,C}$ | Threshold $C^l_L$ for microbial (de)activation | $1.42e^{-5}$ | $9.90e^{-6}$ | $2.19e^{-5}$ | $mol\ C\ cm^{-3}\ water$ |
| $C_{thres,O}$ | | $8.58e^{-6}$ | $7.71e^{-6}$ | $9.76e^{-6}$ | |
| $D_{HW}$ | Diffusion coefficient of high molecular weight organic carbon | $3.456e^{-3}$ | | | $cm^2\ d^{-1}$ |
| $D_{LW}$ | Diffusion coefficient of dissolved low molecular weight organic carbon | 2.07 | 0.92 | 1.45 | $cm^2\ d^{-1}$ |
| $k_{ads}$ | Adsorption rate | $2.7e^{-7}$ | | | $cm^3\ scv\ mol\ C^{-1}\ d^{-1}$ |
| $k_{d,C}$ | Deactivation rate coefficient | 2.73 | 1.49 | 1.37 | $d^{-1}$ |
| $k_{d,O}$ | | 0.24 | 4.04 | 0.11 | |
| $k_{des}$ | Desorption rate | $5e^{-5}$ | | | $d^{-1}$ |
| $k_{C,S}$ | Substrate affinity to dissolved low molecular weight organic C | $4.93e^4$ | $1.50e^5$ | $7.72e^4$ | $mol\ C\ cm^{-3}\ scv$ |
| $k_{O,S}$ | | $1.02e^6$ | $1.16e^7$ | $9.55e^4$ | |
| $K_L$ | Half-saturation coefficients of enzymes targeting HMW | $1.98e^{-6}$ | $1.02e^{-7}$ | $6.23e^{-4}$ | $mol\ C\ cm^{-3}\ scv$ |
| $k_{max,C}$ | Maximum maintenance rate coefficient | $7.07e^{-3}$ | $1.38e^{-3}$ | $1.46e^{-3}$ | $d^{-1}$ |
| $k_{max,O}$ | | $2.30e^{-4}$ | $6.57e^{-4}$ | $1.14e^{-3}$ | |
| $k_{r,C}$ | Reactivation rate coefficient | 86.3 | 95.9 | 54.3 | $d^{-1}$ |
| $k_{r,O}$ | | 1.17 | 54.9 | 0.181 | |
| $v_{max,depoly}$ | Maximum reaction rate of enzymes targeting HMW | 0.108 | $1.31e^{-2}$ | $1.69e^{-3}$ | $d^{-1}$ |

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


**Table A2.** Continued

| Symbol | Definition (and source) | Value per selected parameter set | | | Unit |
|---|---|---|---|---|---|
| | | *highCO2* | *highMB* | *lowMUptake* | |
| $Y$ | Maintenance yield | 0.372 | $2.54e^{-2}$ | 0.397 | – |
| $Y_C$ | Growth yield on dissolved low molecular weight organic carbon | $1.08e^{-2}$ | 0.108 | 0.422 | – |
| $Y_O$ | | $2.43e^{-2}$ | 0.142 | 0.896 | |
| $\alpha$ | Empirical parameter determining the curvature of Eq.D10 (Moyano et al., 2013) | 1.47 | | | – |
| $\beta_C$ | Reduction factor of maintenance requirements in dormant state | $1.64e^{-3}$ | $5.13e^{-3}$ | $1.09e^{-4}$ | – |
| $\beta_O$ | | 0.592 | $9.32e^{-2}$ | $3.31e^{-2}$ | |
| $\mu_{max,C}$ | Maximum growth rate coefficient | 0.83 | 1.42 | 0.25 | $d^{-1}$ |
| $\mu_{max,O}$ | | $1.03e^{-2}$ | $3.56e^{-2}$ | $1.26e^{-2}$ | |
| $\rho_L$ | Proportion of high molecular weight organic carbon formed from dead microbial biomass due to maintenance | $2.16e^{-2}$ | 0.579 | $1.51e^{-2}$ | – |
| $\rho_b$ | Soil bulk density | 1.51 | | | $g\ mineral\ soil\ cm^{-3}\ scv$ |
| $\tau$ | $\tau = \frac{\psi_{m,soil,D2A}}{\psi_{m,soil,A2D}}$, with $\psi_{m,soil,D2A}$ the threshold soil matric potential for microbial activation (Wang et al., 2021) | 0.39 | | | – |
| $\psi_{m,soil,A2D}$ | Threshold soil matric potential for microbial deactivation (Wang et al., 2021) | 4600 | | | $hPa$ |
| $\psi_{m,soil,opt}$ | Threshold soil matric potential above which water is not limiting for microbial activity (Moyano et al., 2013) | $-30$ | | | $hPa$ |
| $\psi_{m,soil,th}$ | Threshold soil matric potential bellow which microbial activity ceases (Moyano et al., 2013) | $-158000$ | | | $hPa$ |
| $\omega_{DA}$ | Empirical exponent for Eqs.D29,D30 (Wang et al., 2021) | 3.38 | | | – |

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$\frac{\partial \theta_i V_{1DS,scv,i}}{\partial t}$ according to $\psi_{x,crit}$ (see Eq. (B12)). We then set a second limitation on the net sink (resp. source) using the maximum potentially available water (resp. space) in the voxel–equal to the water (resp. space) volume at the beginning of the time step and to the maximum amount of water that could be gained (resp. lost) according to the inter-voxel flow at the last time step. The driving equation for the water flow is defined thus at the macroscale (Mai et al., 2019; Koch et al., 2021):

$$\frac{\partial \theta}{\partial t} = K_{sat} \nabla \cdot (\kappa_m (\nabla \psi_{m,3DS} - \nabla \psi_{g,3DS})) + S_{w,root-3DS} \quad \text{for} \quad \Omega \backslash \partial\Omega,\ t > t_0 \tag{B3}$$

$$S_{w,root-3DS} = S_{w,root-3DS,0} \quad \text{at} \quad t = t_0 \tag{B4}$$

A boundary condition completes the model and can represent, for instance, the net gain or loss of water resulting from rainfall and soil evaporation.

### B2 1D axisymmetric soil models

Because of the small radii of the microscale domains, we assume that the gravitational gradient along the radial coordinate is negligible compared with the matric potential gradient: $abs(\frac{\partial \psi_{g,1DS}}{\partial r}) << abs(\frac{\partial \psi_{m,1DS}}{\partial r})$. We thus get (Debnath, 2005, Eq. 1.10.4):

$$\frac{\partial \theta}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (r K_{sat} \kappa_m \frac{\partial \psi_{m,1DS}}{\partial r}) + \frac{1}{r} S_{w,3DS-1DS} \tag{B5}$$

with $r$ $(cm)$ the radial coordinate along the axisymmetric domain, where $r = 0$ corresponds to the center of root segment associated with the microscale soil domain. $r \in [r_{in}, r_{out}]$, with $r_{in}$ $(cm)$ the inner boundary of the domain, corresponding to the root radius, and $r_{out}$ $(cm)$ the outer boundary of the 1D domain.

The water flow at the inner boundary of 1D domain corresponds to $q_{root-soil}$ (see Eq. (3) ). $S_{w,3DS-1DS}$ is obtained from the bulk soil water flow. For the segment $i$ in the voxel $k$:

$$S_{w,1DS-3DS,i} = -\frac{Q_{w,1DS-3DS,i}}{V_{1DS,scv,i}} \tag{B6}$$

$$Q_{w,1DS-3DS,i} = -Q_{w,3DS-3DS,k} \cdot W_w(i,k) \tag{B7}$$

$$W_w(i,k) = \begin{cases} \frac{(\theta_s - \theta_i) V_{1DS,scv,i} + Q_{w,root-soil,i} dt}{\sum_j^n (\theta_s - \theta_j) V_{1DS,scv,j} + Q_{w,root-soil,j} dt} & \text{if} \quad Q_{w,3DS-3DS,k} > 0 \\ \frac{(\theta_i - \theta_r) V_{1DS,scv,i} - Q_{w,root-soil,i} dt}{\sum_j^{nr} (\theta_j - \theta_r) V_{1DS,scv,j} - Q_{w,root-soil,j} dt} & \text{else} \end{cases} \tag{B8}$$

$$V_{1DS,scv,i} = \pi \left(r_{out,i}^2 - r_{in,i}^2\right) L_{r,i} \tag{B9}$$

$$Q_{w,root-soil,i} = q_{w,root-soil,i} 2\pi r_{in,i} L_i \tag{B10}$$

$Q_{w,3DS-3DS,k}$ $(cm^3\ water\ d^{-1})$ corresponds to the net water change in the sub-control volume caused by the exchange with neighbouring voxels. The second element on the right-hand side of Eq. (B7), $W_w$ $(-)$ is a weighting factor dividing the net water flow between the microscale domains of the macroscale voxel $k$. $W_w$ is computed from the maximal potentially

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


available water (resp. space), which is the sum of [a] the net root water release (resp. uptake) over the evaluated period, and [b] the water (resp. air) volume available at the beginning of the evaluated period. In Eq. (B6), the volume of the microscale domain ($V_{1DS,scv}$, $cm^3$ $scv$ ) is used to convert the net water sink from $cm^3$ $water$ $d^{-1}$ to $cm^3$ $water$ $cm^{-3}$ $scv$ $d^{-1}$. $S_{w,1DS-3DS,i}$ is then divided between the 1D segments of the microscale domains using the same weighting method. We obtain the following driving equation for the microscale soil domains (Mai et al., 2019; Koch et al., 2021):

$$r\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial r}(rK_{sat}\kappa_m\frac{\partial\psi_{m,1DS}}{\partial r}) + rS_{w,1DS-3DS} \quad \text{for} \quad r \in ]r_{in}, r_{out}[,\ t > t_0 \tag{B11}$$

$$K_{sat}\kappa_m\frac{\partial\psi_{m,1DS}}{\partial r} =$$

$$max(q_{w,root-soil},\ K_{sat}\kappa_m\frac{(\psi_{crit,x} - \psi_{m,1DS})}{\Delta r_{root-1DS}}) \quad \text{at} \quad r = r_{in} \tag{B12}$$

$$K_{sat}\kappa_m\frac{\partial\psi_{m,1DS}}{\partial r} = 0 \quad \text{at} \quad r = r_{out} \tag{B13}$$

$$S_{w,3DS-1DS} = S_{w,3DS-1DS,0} \quad \text{at} \quad t = t_0 \tag{B14}$$

with $\psi_{crit,x}$ $(hPa)$ the critical (minimum) xylem water potential. Therefore, if both $\psi_{m,soil}$ and $q_{w,root-soil}$ are low, the realised net water uptake might be more limited than prescribed via $q_{w,root-soil}$.

## Appendix C: Soil carbon transport

In the sections below, we present the implementation of the equations given in section 2.2.4 to the 1D axisymmetric and 3D soil domains.

### C1 3D soil model

For the 3D macroscale soil domain, $S_X$ can be computed in two ways:

1. If there are no roots in the voxel $i$ ($len(nr_i) = 0$), $S_X$ corresponds to the sources computed at the voxel scale ($S_{X,3DS}$, $mol$ $cm^{-3}$ $scv$ $d^{-1}$).
2. If there is at least one root in the voxel, $S_X$ corresponds to the sources computed at the microscale ($S_{X,1DS}$, $mol$ $cm^{-3}$ $scv$ $d^{-1}$).

This method is represented by the following equations:

$$S_X = \begin{cases} \frac{1}{V_{3DS}}\sum_{i=1}^{nr_k} V_{1DS}S_{X,1DS} & \text{if} \quad len(nr_k) > 0 \\ S_{X,3DS} & \text{else} \end{cases} \tag{C1}$$

This allows us to achieve similar results at the micro- and macroscales and to profit from the higher resolution of the microscale models, leading to more accurate results in the soil voxels containing roots. $S_{X,1DS}$ is computed similarly to $S_{w,root-3DS}$ (see Eq. (B1)), by computing the mean C variation rate and limiting the sink according to the C potentially available in the voxel. The driving equation for dissolved low molecular weight organic C is (Mai et al., 2019):

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


$$\frac{\partial \theta C_L^l}{\partial t} - K_{sat}\nabla \cdot \left(\kappa_m C_L^l (\nabla \psi_m - \nabla \psi_g)\right) \tag{C2}$$

$$-\nabla \cdot (D_L(\theta,\phi)\nabla C_L^l) - S_L = 0 \text{ for } \Omega \backslash \partial\Omega,\ t > t_0,$$

$$C_L^l = C_{L,0}^l, \text{ at } t = t_0 \tag{C3}$$

For high molecular weight organic C compounds, we have:

$$\frac{\partial \theta C_H^l}{\partial t} - \nabla \cdot (D_H(\theta,\phi)\nabla C_H^l) - S_H = 0$$

$$\text{for } \Omega \backslash \partial\Omega,\ t > t_0, \tag{C4}$$

$$C_H^l = C_{H;0}^l, \text{ at } t = t_0 \tag{C5}$$

For both equation sets, the boundary conditions can be used to represent an input of organic matter in the soil.

### C2 1D axisymmetric soil models

For 1D axisymmetric microscale soil domains, we get (Mai et al., 2019):

$$\frac{\partial \theta C_X^l}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r} r C_X^l \boldsymbol{u}_X + \frac{1}{r}\frac{\partial}{\partial r} r (D_X(\theta,\ \phi)\frac{\partial C_X^l}{\partial r}) \ + S_X + S_{1DS-3DS,X} \tag{C6}$$

$S_{1DS-3DS,X}$ represents the net source of solutes from inter-voxel exchanges at the macroscale. For the segment $i$ in the voxel $k$:

$$S_{1DS-3DS,X,i} = -\frac{Q_{X,1DS-3DS,i}}{V_{1DS,scv,i}} \tag{C7}$$

$$Q_{X,1DS-3DS,i} = -Q_{X,3DS-3DS,k}\, W_X(i,k) \tag{C8}$$

$$W_X(i,k) = \begin{cases} \frac{m_{X,pot,i}}{\sum_j^n m_{X,pot,j}} & \text{if} \quad Q_{X,3DS-3DS,k} < 0 \\ \frac{1/max(m_{X,pot,i},\epsilon)}{(\sum_j^n 1/max(m_{X,pot,j},\epsilon))} & \text{else} \end{cases} \tag{C9}$$

$$m_{X,pot,i} = \theta_i V_{1DS,scv,i} C_{X,i}^l + Q_{X,root-soil,i} dt \tag{C10}$$

$$Q_{X,root-soil,i} = 2\pi r_{in,i} L_i \cdot \begin{cases} q_{exud,i} & \text{if} \quad \text{X is } C_L^l \\ q_{mucil,i} & \text{if} \quad \text{X is } C_H^l \end{cases} \tag{C11}$$

$m_{X,pot}$ $(mol\ C)$ is the potentially available solute content. $Q_{X,3DS-3DS,k}$ $(mol\ C/d)$ corresponds to the net solute transport into the sub-control volume from other soil voxels. The second element of Eq. (C8) is a weighting factor dependent on the solute content of the microscale domains in the voxel. $V_{1DS,scv,i}$ is used to convert the net solute transport from $mol\ d^{-1}$ to $mol\ cm^{-3}\ d^{-1}$. For solutes we could have $m_{X,pot} = 0$, we, therefore, set a minimum value of $\epsilon \approx 0$ when using ${C_{X,pot}^q}^{-1}$ to avoid a division by 0. The same method is used to divide the net sinks between the 1D segments of the microscale domain.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


Eq. (C6) for dissolved low molecular weight organic C gives:

$$
\begin{aligned}
r\frac{\partial \theta C_L^l}{\partial t} - \frac{\partial}{\partial r}(rC_L^l K_{sat}\kappa_m(S_w)\frac{\partial \psi_m}{\partial r}) & \\
-\frac{\partial}{\partial r}r(D_L(\theta,\,\phi)\frac{\partial C_L^l}{\partial r}) & \qquad \text{(C12)}\\
-r(S_L + S_{1DS-3DS,L}) &= 0 \text{ for } \Omega\backslash\partial\Omega,\, t > t_0,\\
K_{sat}\frac{\partial}{\partial r}\left(\kappa_m C_L^l \frac{\partial \psi_m}{\partial r}\right) + \frac{\partial}{\partial r}(D_L(\theta,\,\phi)\frac{\partial C_L^l}{\partial r}) &= q_{exud,1DS-root} \text{ for } r = r_{in}, \qquad \text{(C13)}\\
K_{sat}\frac{\partial}{\partial r}\left(\kappa_m C_L^l \frac{\partial \psi_m}{\partial r}\right) + \frac{\partial}{\partial r}(D_L(\theta,\,\phi)\frac{\partial C_L^l}{\partial r}) &= 0 \text{ for } r = r_{out}, \qquad \text{(C14)}\\
C_L^l &= C_{L,0}^l, \text{ at } t = t_0 \qquad \text{(C15)}
\end{aligned}
$$

Eq. (C6) for high molecular weight organic C compounds gives:

$$
\begin{aligned}
r\frac{\partial \theta C_H^l}{\partial t} - \frac{\partial}{\partial r}r(D_H(\theta,\,\phi)\frac{\partial C_H^l}{\partial r}) & \qquad \text{(C16)}\\
- r(S_H + S_{1DS-3DS,H}) &= 0 \text{ for } \Omega\backslash\partial\Omega,\, t > t_0,\\
\frac{\partial}{\partial r}(D_H(\theta,\,\phi)\frac{\partial C_H^l}{\partial r}) &= q_{mucil,1DS-root} \text{ for } r = r_{in}, \qquad \text{(C17)}\\
\frac{\partial}{\partial r}(D_H(\theta,\,\phi)\frac{\partial C_H^l}{\partial r}) &= 0 \text{ for } r = r_{out}, \qquad \text{(C18)}\\
C_H^l &= C_{H,0}^l, \text{ at } t = t_0 \qquad \text{(C19)}
\end{aligned}
$$

The solute transport at the inner boundary of the domain corresponds to the exchange with the root ( $q_{exud}$ or $q_{mucil}$, see Eq. (16), (20)).

## Appendix D: Soil reactions and microbial pools

Microorganisms can be modeled as a system of ordinary differential equations in time, (Pot et al., 2022), representing the to SOC mineralisaiton and $CO_2$ release caused by microbes (Pagel et al., 2020). We can describe the microbial behaviour by looking at community-level microbial traits (Bardgett and Caruso, 2020): recent studies indicate that soil bacterial communities are dominated by relatively few taxa with strong environmental preferences. Therefore a focus on the functional traits of dominant taxa can improve our understanding.

The equations in this section were adapted from the ones setup by Sırcan et al. (2025). They present the microbe-driven soil reactions. The microbial community is divided in two main groups: oligotrophs (slower development and higher substrate affinity) and copiotrophs (quicker development and lower substrate affinity). The main differences with the equations presented by Sırcan et al. (2025) are the explicit representation of the soil water content and its influence on microbial processes, and the non-instantaneous C sorption. We present below the list of reactions which sum up to $S_{microbe,X}$ for the organic C

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


concentration of dissolved low molecular weight concentration ($C_L^l$) and high molecular weight compounds ($C_H^l$), as well as the connected microbial pools:

$$S_{microbe,L} = S_{depoly} + (1 - p_L)S_{decay} - S_{growth,L} - S_{Muptake,L} \tag{D1}$$

$$S_{microbe,H} = -S_{depoly} + p_L S_{decay} \tag{D2}$$

with $S_{depoly}$ the depolymerisation rate of high molecular weight organic C compounds, $S_{decay}$ the solute gain from microbial decay, $S_{growth,S}$ the dissolved low molecular weight organic C uptake for microbial growth, and $S_{Muptake,L}$ the dissolved low molecular weight organic C uptake for maintenance (all in $mol\ C\ C^{-3}\ scv\ d^{-1}$). $p_L$ $(mol/mol)$ is the proportion of high molecular weight organic C compounds to total C compounds formed from dead microbial biomass due to maintenance.

The reaction rates are dependent on the concentration of microbial pools. Like Pagel et al. (2020), we define four microbial pools in the solid, described by their C concentration in the soil phase $C_Z^Y$ $(mol\ C\ microbes/cm^3\ scv)$. $Y$ stands either for $a$ (active microbes) or $d$ (dormant microbes). $Z$ stands for $O$ (oligotrophes) or $C$ (copiotrophes).

We define their respective variation thus:

$$\frac{\partial C_O^a}{\partial t} = S_{growth,O} - S_{deact,O} + S_{react,O} - \frac{1}{Y_M} S_{Mdecay,O}^a \tag{D3}$$

$$\frac{\partial C_O^d}{\partial t} = S_{deact,O} - S_{react,O} - \frac{1}{Y_M} S_{Mdecay,O}^d \tag{D4}$$

$$\frac{\partial C_C^a}{\partial t} = S_{growth,C} - S_{deact,C} + S_{react,C} - \frac{1}{Y_M} S_{Mdecay,C}^a \tag{D5}$$

$$\frac{\partial C_C^d}{\partial t} = S_{deact,C} - S_{react,C} - \frac{1}{Y_M} S_{Mdecay,C}^d \tag{D6}$$

$S_{growth,Z}$ corresponds to the growth of $C_Z^a$, $S_{decay,Z}^Y$ corresponds to the decay of $C_Z^{Y,s}$, $S_{deact,Z}$ represents the switch of $C_Z^a$ to $C_Z^d$ and $S_{react,Z}$ represents the switch of $C_Z^d$ to $C_Z^a$ . $S_{Mdecay,Z}^Y$ represents the loss of $C_Z^{Y,s}$ C because of maintenance. All rates are in $mol\ C\ cm^{-3}\ scv\ d^{-1}$. $Y_M$ $(-)$ is the maintenance yield. The growth reaction rates are defined thus:

$$S_{growth,L} = \frac{1}{Y_O} S_{growth,O} + \frac{1}{Y_C} S_{growth,C} \tag{D7}$$

$$S_{growth,O} = f_A(\psi_{m,soil}) \frac{\mu_{max,O}\ C_L^l\ k_{O,L}}{\mu_{max,O} + C_L^l k_{O,L}} C_O^a \tag{D8}$$

$$S_{growth,C} = f_A(\psi_{m,soil}) \frac{\mu_{max,C}\ C_L^l\ k_{C,L}}{\mu_{max,C} + C_L^l\ k_{C,L}} C_C^a \tag{D9}$$

$$f_A(\psi_{m,soil}) = \begin{cases} 1, & \psi_{m,soil} > \psi_{m,soil,opt} \\ 1 - \left( \frac{log_{10}(\psi_{m,soil}/\psi_{m,soil,opt})}{log_{10}(\psi_{m,soil,th}/\psi_{m,soil,opt})} \right)^{\alpha}, & \psi_{m,soil} \in [\psi_{m,soil,th}, \psi_{m,soil,opt}] \\ 0, & \psi_{m,soil} < \psi_{m,soil,th} \end{cases} \tag{D10}$$

With $Y_Z$ $(-)$ the growth yield of $C_Z$. $\mu_{max,Z}$ $(1/d)$ is the maximum growth rate of $C_Z^a$. $k_{O,L}$ $(cm^3\ scv\ d\ mol^{-1}\ C)$ is the $C_Z^a$ affinity to $C_L^l$. $f_A(\psi_{m,soil})$ $(-)$ defines the water limitation on the access of the microorganisms and enzymes to the solutes

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


(Moyano et al., 2013). The maintenance decay rates are defined thus:

$$S_{Mdecay} = S^a_{Mdecay,O} + S^d_{Mdecay,O} + S^a_{Mdecay,C} + S^d_{Mdecay,C} \tag{D11}$$

$$S^a_{Mdecay,O} = k_{max,O}\overline{C^a_O} - S^a_{Muptake,L,O} \tag{D12}$$

$$S^d_{Mdecay,O} = k_{max,O}\beta_O C^d_O - S^d_{Muptake,L,O} \tag{D13}$$

$$S^a_{Mdecay,C} = k_{max,C}\overline{C^a_C} - S^a_{Muptake,L,C} \tag{D14}$$

$$S^d_{Mdecay,C} = k_{max,C}\beta_C C^d_C - S^d_{Muptake,L,C} \tag{D15}$$

$$\overline{C^a_O} = max(0., C^a_O - C^a_{O,lim}) \tag{D16}$$

$$\overline{C^a_C} = max(0., C^a_C - C^a_{C,lim}) \tag{D17}$$

$k_{max,Z}$ $(1/d)$ is the maximum maintenance rate coefficient for $C_Z$. $\beta_Z$ $(-)$ is the reduction factor of maintenance requirements in dormant state for $C_Z$. $C^a_{Z,lim}$ $(mol\ C/cm^3\ scv)$ corresponds to the minimal value of $C^a_Z$ below which the microbial pool can only be subjected to growth. This limitation allows us to have a re-development of the pool even if we have no solute in the soil for a period of time. We use consequently the limited $\overline{C^a_Z}$ $(mol\ C/cm^3\ scv)$ value for all reaction rates except for $S_{growth,Z}$. The uptake rates are defined thus:

$$S_{uptake,L} = S^a_{uptake,L,O} + S^d_{uptake,L,O} + S^a_{uptake,L,C} + S^d_{uptake,L,C} \tag{D18}$$

$$S^a_{uptake,L,O} = f_A(\psi_{m,soil})\frac{k_{max,O}C^l_L k_{O,L}}{k_{max,O} + C^l_L k_{O,L}}\overline{C^a_O} \tag{D19}$$

$$S^d_{uptake,L,O} = f_A(\psi_{m,soil})\frac{k_{max,O}C^l_L k_{O,L}}{k_{max,O} + C^l_L k_{O,L}}\beta_O C^d_O \tag{D20}$$

$$S^a_{uptake,L,C} = f_A(\psi_{m,soil})\frac{k_{max,C}C^l_L k_{C,L}}{k_{max,C} + C^l_L k_{C,L}}\overline{C^a_C} \tag{D21}$$

$$S^d_{uptake,L,C} = f_A(\psi_{m,soil})\frac{k_{max,C}C^l_L k_{C,L}}{k_{max,C} + C^l_L k_{C,L}}\beta_C C^d_C \tag{D22}$$

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


The deactivation and reactivation rates are defined thus:

$$S_{deact,O} = \max((1-\phi_O), f_{A2D}(\psi_{m,soil}))k_{d,O}\overline{C_O^a} \tag{D23}$$

$$S_{deact,C} = \max((1-\phi_C), f_{A2D}(\psi_{m,soil}))k_{d,C}\overline{C_C^a} \tag{D24}$$

$$S_{react,O} = \min(\phi_O, f_{D2A}(\psi_{m,soil}))k_{r,O}C_O^d \tag{D25}$$

$$S_{react,C} = \min(\phi_C, f_{D2A}(\psi_{m,soil}))k_{r,C}C_C^d \tag{D26}$$

$$\phi_O = \frac{1}{e^{\frac{C^l_{thres,O}-C^l_L}{aC^l_{thres,O}}}+1} \tag{D27}$$

$$\phi_C = \frac{1}{e^{\frac{C^l_{thres,C}-C^l_L}{aC^l_{thres,C}}}+1} \tag{D28}$$

$$f_{A2D}(\psi_{m,soil}) = \frac{1}{1+[\psi_{m,soil,A2D}/\psi_{m,soil}]^{\omega_{DA}}} \tag{D29}$$

$$f_{D2A}(\psi_{m,soil}) = \frac{1}{1+[\psi_{m,soil}/(\tau\ \psi_{m,soil,A2D})]^{\omega_{DA}}} \tag{D30}$$

with $k_{d,Z}$ and $k_{r,Z}$ $(1/d)$ respectively the deactivation and reactivation rate coefficients for $C_Z$. $C^l_{thres,Z}$ $(mol\ C/cm^3\ water)$ is the $C^l_L$ threshold for $\phi_Z$. $\phi_Z$ $(-)$ is the switch function defining the effect of $C^l_L$ on microbial dormancy ($S_{deact,Z}$ and $S_{react,Z}$), while $f_{A2D}$ and $f_{D2A}$ $(-)$ define the effect of soil water content (see Wang et al. (2021)). The increase of the deactivation (resp. decrease of the activation) is defined by the most limiting resource between dissolved low molecular weight organic C and water. For instance, when water limiting for microbial activation, we will have $\min(\phi_Z, f_{D2A}(\psi_{m,soil})) = f_{D2A}(\psi_{m,soil})$ or $\max((1-\phi_Z), f_{A2D}(\psi_{m,soil})) = f_{A2D}(\psi_{m,soil})$. Finally, we get the depolymerisation rate (Pagel et al., 2020):

$$S_{depoly} = f_A(\psi_{m,soil})v_{max,depoly}\frac{C^l_H}{K_L + C^l_H}\overline{C_O^a} \tag{D31}$$

With $v_{max,depoly}$ $(1/d)$ is the maximum reaction rate of enzymes targeting high molecular weight organic C compounds, $K_L$ $(mol/cm^3\ water)$ half-saturation coefficients of enzymes targeting high molecular weight organic C compounds.

From the reactions defined above, we also get $C_{co2}$ $(mol\ C/cm^3\ scv)$, the amount of C released:

$$\frac{\partial C_{co2}}{\partial t} = \frac{1-Y_O}{Y_O}S_{growth,O} + \frac{1-Y_C}{Y_C}S_{growth,C} + \frac{1-Y_M}{Y_M}S_{Mdecay} + S_{Muptake,L} \tag{D32}$$

Although we do compute the amount of C released, we do not simulate its transport in the domain.

## Appendix E: Growth of existing 1D axisymmetric soil models

Once the 1D domain volumes at time step $N$ have been computed (see Eq. (26)), the redistribution of the water and C between the microscale domains of a voxel are done in 2 steps:

1. Compute the new water volume and solute content in the pre-existing microscale domains that have shrunk while trying to maintain the radial concentration gradients.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


2. Compute the water volume and C content of the new microscale domains and of the pre-existing microscale domaines that have grown. We define for each voxel a mean water content and C concentration from the leftover water volume, C content, and voxel space. There is no concentration gradient in the newly added microscale space.

We set $m_X$ $(mol)$ as the content of the C element $X$ with the concentration $C_X$, and $V_w$ $(cm^3\ water)$ the water volume.

### E1 Shrinking 1D axisymmetric soil models

For perirhizal zone with a volume decrease between time step $N-1$ and $N$, we adapt $m_X$ in each soil voxel so that, for the segment $k$:

$$\textit{ChangeRatioS}_k = \frac{m_{x,k}^N}{m_{X,k}^{N-1}}$$

$$\textit{ChangeRatioW}_k = \frac{V_{w,k}^N}{V_{w,k}^{N-1}}$$

We set *ChangeRatioS* and *ChangeRatioW* so that the microscale domain will lose or gain water and solute according to the volume change. *ChangeRatioW* is also adapted to keep $\theta \in [\theta_{wiltingpoint}, \theta_s]$. $\theta_{wiltingpoint}$ is the soil water content when $\psi = \psi_{crit}$ the critical plant water potential. Consequently:

$$\textit{ChangeRatioS}_k = min(\frac{V_{1DS,scv,k}^N}{V_{1DS,scv,k}^{N-1}}, 1) \tag{E1}$$

$$\textit{ChangeRatioW}_k = max(min(\textit{ChangeRatioS}_k, \frac{\theta_s\ V_{1DS,scv,k}^N}{V_{w,k}^{N-1}}), \frac{\theta_{wiltingpoint}\ V_{1DS,scv,k}^N}{V_{w,k}^{N-1}}) \tag{E2}$$

We also want to keep the radial concentration gradients:

$$\frac{\partial C_k^N}{\partial r} = \frac{\partial C_k^{N-1}}{\partial r} \tag{E3}$$

$$\frac{\partial \theta_k^N}{\partial r} = \frac{\partial \theta_k^{N-1}}{\partial r} \tag{E4}$$

For the discretised microscale domain made of $n$ segments, this gives us a set of equations that can be solved analytically. In matricial form:

$$\mathcal{B} = Q^{-1}G \tag{E5}$$

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


With $Q$ a matrix of size $[n, n]$ :

$$Q = \begin{bmatrix} -1 & 1 & 0 & ... & 0 \\ 0 & -1 & 1 & ... & 0 \\ 0 & ... & ... & ... & 0 \\ 0 & ... & ... & -1 & 1 \\ V_{0,k}^N & V_{1,k}^N & ... & V_{n-1,k}^N & V_{n-1,k}^N \end{bmatrix} \tag{E6}$$

And $G$ an array of size $n$:

$$G = \begin{bmatrix} b_{r_{1,k}^N}^{N-1} - b_{r_{0,k}^N}^{N-1} \\ ... \\ ... \\ b_{r_{n,k}^N}^{N-1} - b_{r_{n-1,k}^N}^{N-1} \\ B_k^{N-1} \mathit{ChangeRatio}_k^N \end{bmatrix} \tag{E7}$$

$B_k^N$ is the total amount of the solute or of water (in $mol$ or $cm^3$) and $b$ is the solute concentration or water content. The last lines of $G$ and $Q$ assure that we obtain the correct total solute and water amount, the other lines represent the wished for gradient between the new location of the segment centers. The value of $b_{r_{1,k}^N}^{N-1} - b_{r_{0,k}^N}^{N-1}$ give the changes of $b$ (at $N-1$) between the segment centers (distance at $N$). It is obtained by interpolation of the concentration gradients between the segments centers at the end of time step $N-1$.

*ChangeRatioW*$_k$ and *ChangeRatioS*$_k$ ensure that the overall $\theta$ and $m_k$ in the whole microscale domain remains within the needed range, but not for each segment. Consequently, when implementing the new water value for each microscale segment, we adapt the distribution of the water between the segments to have for each segment $\theta \in [\theta_{wiltingpoint}, \theta_s]$. Likewise, we ensure that $min(m_k) \geq 0$.

This yields $C_{1DS}^{N,0,-1}$ and $\theta_{1DS}^{N,0,-1}$ to be used at the beginning of the next fixed point loop iteration, see section F.

### E2 New and expanding 1D axisymmetric soil models

From the concentration of the existing microscale domains per voxel, we compute the mean $\theta_{new}$ and $C_{new}$, the water and concentration in the newly freed soil space. $\theta_{new}$ and $C_{new}$ will define the initial conditions of the added volume in the expanding or new microscale domains. For this, we compute the total volume of the newly freed volume in the voxel ($V_{3DS,scv,leftover}^N$, $cm^3$):

$$V_{3DS,scv,i,leftover}^N = \sum_j^{nr_{shrunk,i}^N} L_{j,N} \pi ({r_{out,j}^N}^2 - r_{in,j}^2) \tag{E8}$$

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


with $nr^N_{shrunk,i}$ the sets of microscale domains in voxel $i$ that have shrunk at time step $N$. We then get the content of water and C that are not in the old microscale domains of voxel $i$ anymore:

$$V^N_{3DS,w,i,leftover} = \sum_{j}^{nr^N_{shrunk,i}} V^{N-1}_{1DS,w,j} - V^N_{1DS,w,j} \tag{E9}$$

$$m^N_{3DS,X,i,leftover} = \sum_{j}^{nr^N_{shrunk,i}} m^{N-1}_{1DS,X,j} - m^N_{1DS,X,j} \tag{E10}$$

We can then get $\theta_{new}$ and $C_{new}$:

$$\theta^N_{k,new} = \begin{cases} \frac{V^N_{3DS,w,i,leftover}}{V^N_{3DS,scv,i,leftover}} & \text{if} \quad len(nr^{N-1}_i) > 0 \\ \frac{V^{N-1}_{3DS,w,i}}{V^{N-1}_{3DS,scv,i}} & \text{else} \end{cases} \tag{E11}$$

$$C^{y,N}_{k,new} = \begin{cases} \frac{X^N_{i,leftover}}{V^N_{3DS,i,leftover}} & \text{if} \quad len(nr^{N-1}_i) > 0 \\ \frac{X^{N-1}_i}{V^{N-1}_{3DS,i}} & \text{else} \end{cases} \tag{E12}$$

$$V_{3DS,i,leftover} = \begin{cases} V_{3DS,w,i,leftover} & \text{if} \quad C^y = C^l \\ V_{3DS,scv,i,leftover} & \text{if} \quad C^y = C^s \end{cases} \tag{E13}$$

$$V_{3DS,i} = \begin{cases} V_{3DS,w,i} & \text{if} \quad C^y = C^l \\ V_{3DS,scv,i} & \text{if} \quad C^y = C^s \end{cases} \tag{E14}$$

We can then add the C and water to the growing microscale domains (the C concentration is null for newly created domains):

$$\theta^{N,0,-1}_{1DS} = \theta^{N-1}_{1DS} + \theta^N_{k,new} \Delta V_{1DS,scv,k} \tag{E15}$$

$$C^{N,0,-1}_{1DS} = C^{N-1}_{1DS} + C^N_{k,new} \Delta V_{1DS,scv,k} \tag{E16}$$

We then use the method presented in section E1 to obtain the $\theta$ and $C_X$ value for each microscale segment respecting the new content and trying to maintain the old concentration gradients. This yields $C^{N,0,-1}_{1DS}$ and $\theta^{N,0,-1}_{1DS}$ to be used at the beginning of the next fixed point loop iteration, see section F.

## Appendix F: Pseudo-code of the iterative computation loop

The three models (plant, 1D microscale soil, 3D macroscale soil) are coupled using an iterative approach based on the method Jorda Guerra et al. (2021). In the following section, we present the implementation of the equations defined above, in matricial form and for one time step $N$. Although the water and C balances are computed together, for clarity, the descriptions of their respective computation loops are presented separately.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


## F1 Definition of matrices

For the section below, $M$ represents a matrix of size $[ns,\ nr]$, with $ns$ the number of soil voxels and $nr$ the number of root segments belowground (equal to the number of microscale domains). Other variables include vectors of size $nr$ with root, root-soil interface or microscale soil values (with respectivelly the subscripts $root$, $rsi$, $1DS$). The root-soil interface corresponds to the 1D segment at the inner boundary of the microscale models. Vectors with the subscript $3DS$ give the macroscale soil values and are of size $ns$. $V_{V,w}$ $(cm^3\ water)$, $\theta$, $\psi$, $C_X$ and $\mathbf{m_x}$ $(mol\ C)$, $K_{sri}$ $(cm^2\ hPa^{-}1\ d^{-1})$ are vectors giving respectively the water volume, water content, water potential, component concentration, component content, and hydraulic conductivity at the soil-root interface. $V_{surf,out}$ $(cm^2)$ is a vector of size $nr$ and $V_{surf,out}[i] = 2\pi\ r_{out,i}\ L_{r,i}$ , giving the surface at the outer boundary of the perirhizal zone $i$. Similarly, $V_{surf,in}[i] = 2\pi\ r_{in,i}\ L_{r,i}$ gives the surface at the inner boundary. $V_{V,scv,3DS}$ (resp. $V_{V,scv,1DS}$ ) is a vector of size $ns$ (resp. $nr$) giving the volume of each voxel (resp. of each microscale domain). The source vector is obtained from $\mathbf{S} = SV_V$ and is thus in $cm^3\ water\ d^{-1}$ or in $mol\ d^{-1}$. $M_c$ is a binary matrix. $M_c$ is filled with 0 except for $M_c[i,\ j] = 1$, when the $j^{th}$ root segment (and corresponding 1D soil domain) is in the $i^{th}$ soil voxel. $V_{hasRoot}$ is a vector of size $ns$ with 1 for the macroscale soil voxels with at least one root and 0 elsewhere. We set:

$$M_{surf,in} = M_c \circ V_{surf,in}$$

with $\circ$ the hadamard product and $M_{surf,in}$ a matrix of size $[ns,\ nr]$ giving the inner surface of the microscale domain for each soil voxel. $Q_{w,3DS-3DS}$ $(cm^3\ water\ d^{-1})$, and $Q_{X,3DS-3DS}$ $(mol\ C\ d^{-1})$ are vectors of size $ns$ giving, for all the voxels containing at least one root, the changes in water or C (for a specific component)caused by exchanges with other voxels (i.e., not caused by input from a root or from biochemical reactions). $M_{weight,X}$ is the weight matrices used to divide voxel flows ($Q_{3DS-3DS}$ ) between the microscale domains in each voxel (see Eq. (B8),(C9))

## F2 Fixed point iteration for the water flow

The pseudo-code below presents the implementation of the fixed-point iteration loop for the water flow.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


(A) $L^N_{root}, M^N_c = \mathbf{Growth}(\text{Env}^N, \mathbf{C}^{st,N-1}_L, \psi^{N-1}_x)$

$M^N_{surf,in}, V^N_{surf,in}, V^N_{surf,out}, \theta^{N,0,-1}_{1DS}, \psi^{N,0,-1}_{rsi} =$

$\mathbf{Distribute}(L^N_{root}, M^N_c, \theta^{N-1}_{1DS})$

$Q^{N,0,-1}_{w,3DS} = Q^{N-1}_{w,3DS}, \theta^{N,0,-1}_{3DS} = \theta^{N-1}_{3DS}$ (F1)

for $n$ in range($\frac{\Delta t}{\delta t}$):

while any(err$_{...}$ $>$ $\epsilon_{...}$), and $k < k_{max}$:

(B) $q^{N,n,k}_{w,root-soil}, \psi^{N,n,k}_x = \mathbf{FlowPhoto}(\text{Env}^{N,n}, \psi^{N,n,k-1}_{rsi})$ (F2)

(C) $S^{N,n,k}_{w,1DS-3DS} = -M^{N,n,k,T}_{weight,w} Q^{N,n,k-1}_{w,3DS}$ (F3)

$K^{N,n,k}_{sri}, \theta^{N,n,k}_{1DS}, q^{N,n,k,limited}_{w,root-soil} = \mathbf{Flow}(V^N_{surf,in} q^{N,n,k}_{w,root-soil} \delta t,$

$\mathbf{S}^{N,n,k}_{w,1DS-3DS} \delta t, \theta^{N,n,k-1}_{1DS}, V^N_{V,scv,1DS})$ (F4)

$\mathbf{S}^{N,n,k}_{w,3DS} = M^N_{surf,in} q^{N,n,k,limited}_{w,root-soil}$ (F5)

(D) $\theta^{N,n,k}_{3DS}, Q^{N,n,k}_{w,3DS} = \mathbf{Flow}(\mathbf{S}^{N,n,k}_{w,3DS} \delta t, \theta^{N,n,k-1}_{3DS}, V_{V,scv,3DS})$ (F6)

(E) $\text{errW}^{N,n,k}_{1DS,3DS,cumul} = \mathbf{Err}(M_c[\theta^{N,n,k}_{1DS} V^N_{V,scv,1DS}] -$

$[\theta^{N,n,k}_{3DS} V_{V,scv,3DS}])$ (F7)

$\text{errW}^{N,n,k}_{1DS,3DS} = \text{errW}^{N,n,k}_{1DS,3DS,cumul} - \text{errW}^{N,n-1}_{1DS,3DS,cumul}$ (F8)

$\text{errW}_{k,k-1} = \mathbf{Err}(X^{N,n,k} - X^{N,n,k-1})$ (F9)

$\text{errW}_{qroot} = \mathbf{Err}(q^{N,n,k,limited}_{w,root-soil} - q^{N,n,k}_{w,root-soil})$ (F10)

$\text{errW}_{mass1DS} = \mathbf{Err}(\theta^{N,n,k}_{1DS} V^N_{V,scv,1DS} - [\theta^{N,n,IC}_{1DS} V^N_{V,scv,1DS} +$

$(V^N_{surf,in} q^{N,n,k}_{w,root-soil} + \mathbf{S}^{N,n,k}_{w,1DS-3DS} S^{N,n,k}_{w,1DS-1DS}) \Delta t])$ (F11)

$\text{errW}_{mass3DS} = \mathbf{Err}(\sum^{segments} (\theta^{N,n,k}_{3DS} V_{V\,scvw,3DS} - [\theta^0_{3DS} V_{V,scv,3DS}$

$+ \sum^{N}_{j} (M^j_{surf,in} q^j_{w,root-soil} \delta t^j)]))$ (F12)

assert err$_{...} \leq \epsilon_{...}$ (F13)

$\psi^{N,n+1,-1}_{rsi} = \psi^{N,n,k}_{rsi}, \theta^{N,n+1,-1}_{1DS} = \theta^{N,n,k}_{1DS}$

$Q^{N,n+1,-1}_{w,3DS} = Q^{N,n,k}_{w,3DS}, \theta^{N,0,-1}_{3DS} = \theta^{N-1}_{3DS}$ (F14)

$N$ (resp. $\Delta t$) is the step index (resp. time step) of the whole computation loop and $n$ (resp. $\delta t$) is the step index (resp. time step) of the fixed point iteration. $k$ is the iteration number of the fixed point iteration and $k_{max}$ the maximum amount of iteration allowed. Env represents other environmental conditions, $L_{root}$ $(cm)$ is a vector which contains the length of each root segment (and thus microscale domain).

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


The $T$ superscript gives the transpose of a matrix. $\mathbf{Flow}$ represents a function computing the water flow and $\mathbf{FlowPhoto}$ the coupled plant water flow and photosynthesis. $\mathbf{Distribute}$ corresponds to the division of the voxel volume and water between the microscale domains according to the methods presented in section 2.2.6. $\text{err}_{1DS,3DS,cumul}$ gives the difference between the water content values computed at the micro- and macroscale and $\text{err}_{1DS,3DS}$ the difference added at the last time step. $\text{err}_{qroot}$ is the difference between the root water uptake rates computed by the plant and the microscale soil. $\text{err}_{mass}$ gives the mass balance error, $\text{err}_{k,k-1}$ the output differences between the last two iterations (non-convergence). $\mathbf{Err}$ is a function to sum and normalise the error. $\text{err}_{...}$ corresponds to each of the errors computed within the iteration loop, and $\epsilon_{...}$ is their respective maximum value allowed.

### F3 Fixed point iteration for the solutes transport

The pseudo-code below presents the implementation of the fixed-point iteration loop for the C transport.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


(A) $L^N_{root}, M^N_c, q^N_{X,root-soil}, C^{st,N}_{X,root} = \mathbf{Growth} \circ \mathbf{TransportReac}(\text{Env}^N, \sum_j^n (A^{N-1,j}_n \delta t^{N,j}), C^{N-1}_{X,rsi})$ (F15)

$M^N_{surf,in}, V^N_{surf,in}, V^N_{surf,out}, C^{N,0,-1}_{X,1DS} = \mathbf{Distribute}(L^N_{root}, M^N_c, C^{N-1}_{X,1DS})$ (F16)

$Q^{N,0,-1}_{X,3DS} = Q^{N-1}_{X,3DS}, C^{N,0,-1}_{X,3DS} = C^{N-1}_{X,1DS}$ (F17)

for $n$ in range($\frac{\Delta t}{\delta t}$):

while any(err$_{...}$ $>$ $\epsilon_{...}$), and $k < k_{max}$:

(B) $q^{N,n,k}_{X,root-soil}, A^{N,n,k}_n = \mathbf{TransportPhoto}(\text{Env}^{N,n}, \psi^{N,n,k-1}_{rsi})$ (F18)

(C) $\mathbf{S}^{N,n,k}_{X,1DS-3DS} = -M^{N,n,k,T}_{weight,X} Q^{N,n,k-1}_{X,3DS}$ (F19)

$C^{N,n,k}_{X,1DS}, \mathbf{m}^{N,n,k}_{X,1DS} = \mathbf{TransportReac}(V^N_{surf,in} q^N_{X,root-soil} \delta t, \mathbf{S}^{N,n,k}_{X,1DS-3DS} \delta t, C^{N,n,k}_{X,1DS}, \theta^{N,n,k}_{1DS})$ (F20)

$\mathbf{S}^{N,k}_{X,3DS} = M^N_c((\mathbf{m}^{N,n,k}_{X,1DS} - \mathbf{m}^{N,n-1}_{X,1DS})/\delta t + \mathbf{S}^{N,n,k}_{X,1DS-3DS})$ (F21)

(D) $C^{N,n,k}_{X,3DS}, Q^{N,n,k}_{X,3DS} = V_{hasRoot} \mathbf{Transport}(\mathbf{S}^{N,n,k}_{X,3DS} \delta t, \mathbf{C}^{N,n-1}_{X,3DS}) + (1 - V_{hasRoot}) \mathbf{TransportReac}(\mathbf{C}^{N,n-1}_{X,3DS})$ (F22)

(E) $\text{errC}_{1DS,3DS,cumul} = \mathbf{Err}(M^N_c \mathbf{m}^{N,k}_{\mathbf{x}1DS} - \mathbf{m}^{N,k}_{\mathbf{x}3DS})$ (F23)

$\text{errC}^{N,n,k}_{1DS,3DS} = \text{errC}^{N,n,k}_{1DS,3DS,cumul} - \text{errC}^{N,n-1}_{1DS,3DS,cumul}$ (F24)

$\text{errC}_{k,k-1} = \mathbf{Err}(X^{N,n,k} - X^{N,n,k-1})$ (F25)

$\text{errC}_{mass1DS} = \mathbf{Err}(\sum_{comp}^{NComp} (\mathbf{m}^{N,k}_{X,1DS} - [\mathbf{m}^{N-1}_{X,1DS} + (V^N_{surf,in} q^{N,k}_{X,root-soil} + S^{N,k}_{x,1DS-1DS} + S^{N,k}_{x,1DS-3DS}) \Delta t]))$ (F26)

$\text{errC}_{mass3DS} = \mathbf{Err}(\sum^{segments} (\sum_{comp}^{NComp} (\mathbf{m}^N_{X,3DS} - [\mathbf{m}^0_{X,3DS} + \sum_n^N M^n_{surf,in} q^n_{X,root-soil} \Delta t)]))$ (F27)

assert err$_{...} \leq \epsilon_{...}$ (F28)

$\mathbf{m}^{N,n+1,-1}_{X,1DS} = \mathbf{m}^{N,n,k}_{X,1DS}, C^{N,n+1,-1}_{X,1DS} = C^{N,n,k}_{X,1DS}$ (F29)

$Q^{N,n+1,-1}_{X,3DS} = Q^{N,n,k}_{X,3DS}, C^{N,n+1,-1}_{X,3DS} = C^{N,n,k}_{X,3DS}$ (F30)

**TransportReac** represents the implementation of a function computing biochemical reactions and solute transport according to input variables. We need to sum all the components for the solute mass balance ($err_{mass}$). $A_n$ is the net assimilation of

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


sucrose, thus $A_n \neq 0$ only for dissolved low molecular weight organic C ($C_L^l$ and $\mathbf{m}_L$). $Q_{X,3DS} \neq 0$ only for the C of dissolved low molecular weight organic compounds and high molecular weight organic compounds.

## Appendix G: Soil parameters and process constraints

The tables below present the parameter and process constraints defined for TraiRhizo by Sırcan et al. (2025). Baseline soil corresponds to the soil outside the rhizosphere.

**Table G1.** Parameter constraints defined by Sırcan et al. (2025)

| | Constraint | Description/ Explanation |
|---|---|---|
| 1 | $\mu_{max,C} > \mu_{max,O}$ | Maximum growth rate of copiotrophs is higher than maximum growth rate of oligotrophs. |
| 2 | $k_{O,S} > k_{C,S}$ | Specific substrate affinity to small molecules for oligotrophs is higher than for copiotrophs. |
| 3 | $k_{max,C} > k_{max,O}$ | Maximum maintenance rate coef. must be higher for copiotrophs than for oligotrophs. |
| 4 | $C_{thresh,C} > C_{thresh,O}$ | Oligotrophs (K-strategists) are adapted to low carbon and nutrient availability. |
| 5 | $k_{max,i} < \mu_{max,i}$ $i \in \{O,C\}$ | It is a logical constraint to ensure organisms "fit to survive". |
| 6 | $k_{r,i} \geq k_{d,i}$ $i \in \{O,C\}$ | Transition to dormant (or potentially active) state is typically slower than reactivation. |
| 7 | $k_{j,i} > \mu_{max,i}$ $i \in \{O,C\}, j \in \{r,d\}$ | Changes of metabolic state are faster than growth, death, and changes in composition |
| 8 | $Y_O > Y_C$ | Oligotrophs are slow growing at high yield, copiotrophs are fast-growing at low yield |

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


**Table G2.** Process constraints adapted from the ones defined by Sırcan et al. (2025). [a]: The lower bound of the constraints was decreased by 10% compared with the value defined by Sırcan et al. (2025). [b]: The lower bound of the constraints was decreased by 10% compared with the value defined by Sırcan et al. (2025).

| | Constraint | Description/ Explanation |
|---|---|---|
| 1 | $3.33e^{-6} < (C_O + C_C)_R < 1e^{-4}\ mol\ cm^{-3}$ | The range for the concentration of microbial biomass in the rhizosphere from literature for different soil types, textures, experimental conditions. |
| 2[a] | $0.9 < (\frac{(C_O+C_C)_R}{(C_O+C_C)_B} < 2.5$ | Microbial biomass is higher in the rhizosphere than baseline soil and lower than a threshold value which is set up from literature. |
| 3[b] | $3.33e^{-4} < (C_L^l + C_H^l)_R < 1.33e^{-3} \times 1.1\ mol\ cm^{-3}$ | The range for soil organic carbon in the rhizosphere for different soil types, textures, experimental conditions. |
| 4[b] | $0.66 < \frac{(C_L^l+C_H^l)_R}{(C_L^l+C_H^l)_B} < 2 \times 1.1$ | The range for ratio of soil organic carbon in the rhizosphere to baseline soil for different soil types, textures, experimental conditions. |
| 5 | $6e^{-4} < (\frac{C_O^a+C_C^a}{C_O+C_C})_R < 0.6$ | The range for ratio of active microbial biomass to total microbial biomass for different soil types, textures, experimental conditions. |
| 6 | $C_{L,R}^l < 4.58e^{-5}\ mol\ cm^{-3}$ | Based on water extractable organic carbon measurements. Water extractable organic carbon should include dissolved organic carbon (DOC) together with some sorbed carbon mass therefore it must be higher than the DOC concentration. |
| 7[a] | $0.9C_{L,B}^l < C_{L,R}^l$ | Based on water extractable organic carbon measurements. |
| 8[a] | $0.9C_{C,R} > C_{O,R}$ | The rhizosphere is dominated by copiotrophs. |
| 9 | $\frac{C_{C,B}}{C_{O,B}} < \frac{C_{C,R}}{C_{O,R}}$ | |

## Appendix H: Lateral root water conductivity in the mature root zone

The mature root area as well as the root water conductivity ($k_{lat,x}$, $cm\ hPa^{-1}\ d^{-1}$) values for the immature zone are taken from Giraud et al. (2023). However, in that study, $k_{lat,x} = 0$ in the mature root area (more than $0.8\ cm$ away from the root

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


tip). To obtain more realistic results, we used the work of Bramley et al. (2007) to evaluate the $\frac{k_{lat,x,mature}}{k_{lat,x,immature}}$ ratio. Bramley et al. (2007, Fig. 4.15) defines the surface-normalised root resistance $k_{tot,x}$ in $m\ s^{-1}\ MPa\ 10^{-8}$ over the length $l$ $(m)$ from the tip as: $k_{tot,x}(l) = (-83 \times l + 20.9) \times 1e-8$ and the mean root conductance (in in $m^3\ s^{-1}\ MPa\ 10^{-11}$) as $K_{tot,x}(l) = (0.7 \times l + 2.4) \times 1e-11$. We can therefore obtain the side surface of the root segment ($A$ in $m$) up to $l$ $cm$ from $A(l) = \frac{K_{tot,x}(l)}{k_{tot,x}(l)}$. Moreover, in their study, the root axial resistance was found to be negligible, and we get therefore $k_{lat,x}(l) = k_{tot,x}(l)$ and $K_{lat,x}(l) = K_{tot,x}(l)$. We assumed that the mean $k_{lat,x}$ over the assumed immature root zone could be defined as $k_{lat,x,immature} \approx k_{lat,x}(0.008)$. We then evaluated $K_{lat,x}$ between $l_1 = 0.07\ m$ from the tip and $l_2 = 0.18\ m$ from the tip, which were the range of distances used in their study. We then computed $\int_{l1}^{l2} A(l)dl$ and $\int_{l1}^{l2} K_{lat,x}(l)dl$. From this we could get $\int_{l1}^{l2} k_{lat,x}(l)dl = \frac{\int_{l1}^{l2} K_{lat,x}(l)dl}{\int_{l1}^{l2} A(l)dl}$. This yielded $\frac{k_{lat,x,mature}}{k_{lat,x,immature}} = \frac{\int_{l1}^{l2} k_{lat,x}(l)dl}{k_{lat,x}(0.008)} \times 100 = 1.45\% \approx 1.5\%$. We consequently set $k_{lat,x,mature} = 0.015 k_{lat,x,immature}$ for our modelling study.

## Appendix I: Calibration of the soil carbon dynamic

This section describes the method used to calibrate the soil C dynamic. The objective was to implement a simple method allowing us to select sets representing different dynamics. A summary of the characteristics of each of the three selected microbial parameter sets is given in table 1.

### I1 Selection of the TraiRhizo parameter sets

In their study, Sırcan et al. (2025) defined 1650 parameter sets for TraiRhizo model according to a series of parameter and process constraints, which are given in appendix G. The 1650 parameter sets were divided in three groups according to the resulting gradients of $C_L^l$ directly at the root surface—small, medium, or strong gradient. [a] We randomly selected 33 sets in each of the three gradient categories. Then, we ran the coupled model on the (adapted) parameterised plant of Giraud et al. (2023) between days 10 and 14 of growth (with dynamic soil water and C flows). [b] Sets that did not respect the process constraints defined by Sırcan et al. (2025) were removed–see Table G2. [c] From the 12 remaining sets, we selected three sets representing different soil C dynamics. For step [a], we ran the simulation without water scarcity effect–meaning, without implementing the effect of water on microbial (de)activation (Eq. (D29), (D30)) and access to soil solutes (Eq. (D10)). For step [b], following the method of (Sırcan et al., 2025) and the analysis of Kuzyakov and Razavi (2019), we defined the rhizosphere as the soil volume up to 3 $mm$ from the root surface. The baseline soil (soil outside of the rhizosphere) values were taken from the macroscale voxel data at the bottom of the soil column. We retained the sets that respected all the constraints for all the rhizosphere units at the end of the simulation. In some cases, some perirhizal zone units were slightly outside the constraints' bounds. To retain those sets, some constraint bounds were enlarged by $10\%$. These bounds-relaxations are indicated in table G2.

Figure I1 gives the concentration of different C pools along the soil depth. The first set led to a high $CO_2$ production in spite of a low microbial development, and was named *highCO2*. The second set led to a high development of the microbial biomass and was named *highMB*. The last set led to low solute mineralisation and microbial development. It was named *lowMUptake*.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


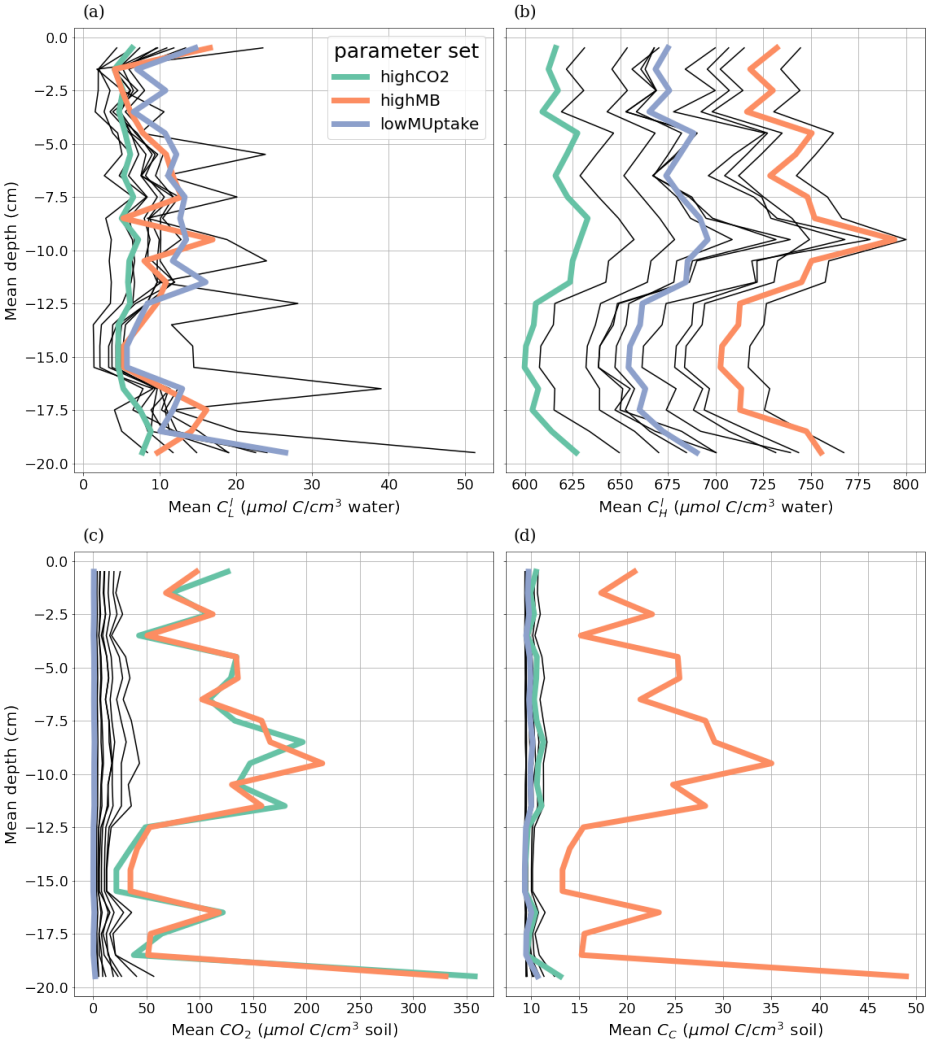


**Figure I1. Mean carbon concentration per soil** after four days of simulation (day 10 to 14) for concentrations of carbon from high ($C_H^l$) and dissolved low ($C_L^l$) molecular weight organic compounds, emitted $CO_2$, and copiotroph carbon ($C_C$), in the 3D soil voxels which contain at least one root segment (perirhizal zone). The line colour gives the index of the parameter set. Only parameter sets that respect the process constraints defined by Sırcan et al. (2025) after four simulation days are represented. The selected sets are *highCO2* (green line), *highMB* (orange line) and *lowMUptake* (purple line).

## I2 Description of the selected TraiRhizo parameter sets

### I2.1 Distribution of the parameter values

Figs. I2 and I3 present frequency histograms for each of the parameters in the 1650 sets. The parameters pointed by the numbered arrows correspond to the parameters of the three selected sets (*highCO2*, *highMB*, *lowMUptake*). As we can see,

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


several of the parameter distributions are strongly skewed to the right, making some of the higher values outliers. Therefore, the sets containing the higher parameter values are more likely to give different outputs when compared with the other sets. From the parameter values, we can give a description of the selected sets:

All three parameter sets offer low $\beta_C$ (activity of dormant copiotrophs), $k_{C,S}$ (copiotroph affinity to dissolved low molecular weight organic C compounds), $k_{d,C}$, $k_{d,O}$ (deactivation rates), $k_{max,C}$, $k_{max,O}$ (maintenance rates), $\mu_{max,C}$, $\mu_{max,O}$ (growth rates), $v_{max,depoly}$ (depolymerisation rates of high molecular weight organic C compounds) values. This follows the average values of the 1650 sets and lead to a lower microbial activity and slower deactivation. Moreover, the sets have higher than average $D_{LW}$ values, which should smooth the distribution of $C_L^l$. As can be seen more clearly in Fig. I3, we have an equilibrium between $k_{d,O}$ and $k_{r,O}$: the sets with higher $k_{d,O}$ also have higher $k_{r,O}$. All sets have a higher $k_{r,C}$ leading to a quick reactivation rate of the copiotrophs. Finally, the three sets have similar $C_{init}^l$ values, and, in particular, a higher than average $C_{L,init}^l$.

*highCO2* stands out by its higher $\beta_O$ value, leading to a higher activity for dormant oligotrophs. Moreover, this sets has the higher $D_{LW}$ values. Finally, the low growth yield ($Y_C$, $Y_O$) may lead to higher C usage and $CO_2$ emission rates.

*highMB* has higher activation rate parameters ($k_{r,O}$, $k_{r,C}$) linked with low $C_{thres}$ parameters, which should lead to a high activated-to-total microbial biomass, although the deactivation parameter for oligotrophs ($k_{d,O}$) is also high. The relatively higher affinity parameters ($k_{C,S}$, $k_{O,S}$) and growth parameters ($\mu_{max,C}$, $\mu_{max,O}$) should lead to a quicker increase of the microbial biomass. The low $Y$ (yield parameters) should also lead to higher C usage and $CO_2$ emissions.

*lowMUptake* stands out for its low activation rate parameters ($k_{r,O}$, $k_{r,C}$) linked with high $C_{thres}$ parameters, which should lead to a high activated-to-total microbial biomass, although the deactivation parameters ($k_{d,C}$, $k_{d,O}$) are also low. Low maintenance need for dormant microbes ($\beta_C$, $beta_O$) and high yield parameters ($Y$, $Y_C$, $Y_O$) should also lead to a lower C usage and $CO_2$ emissions.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


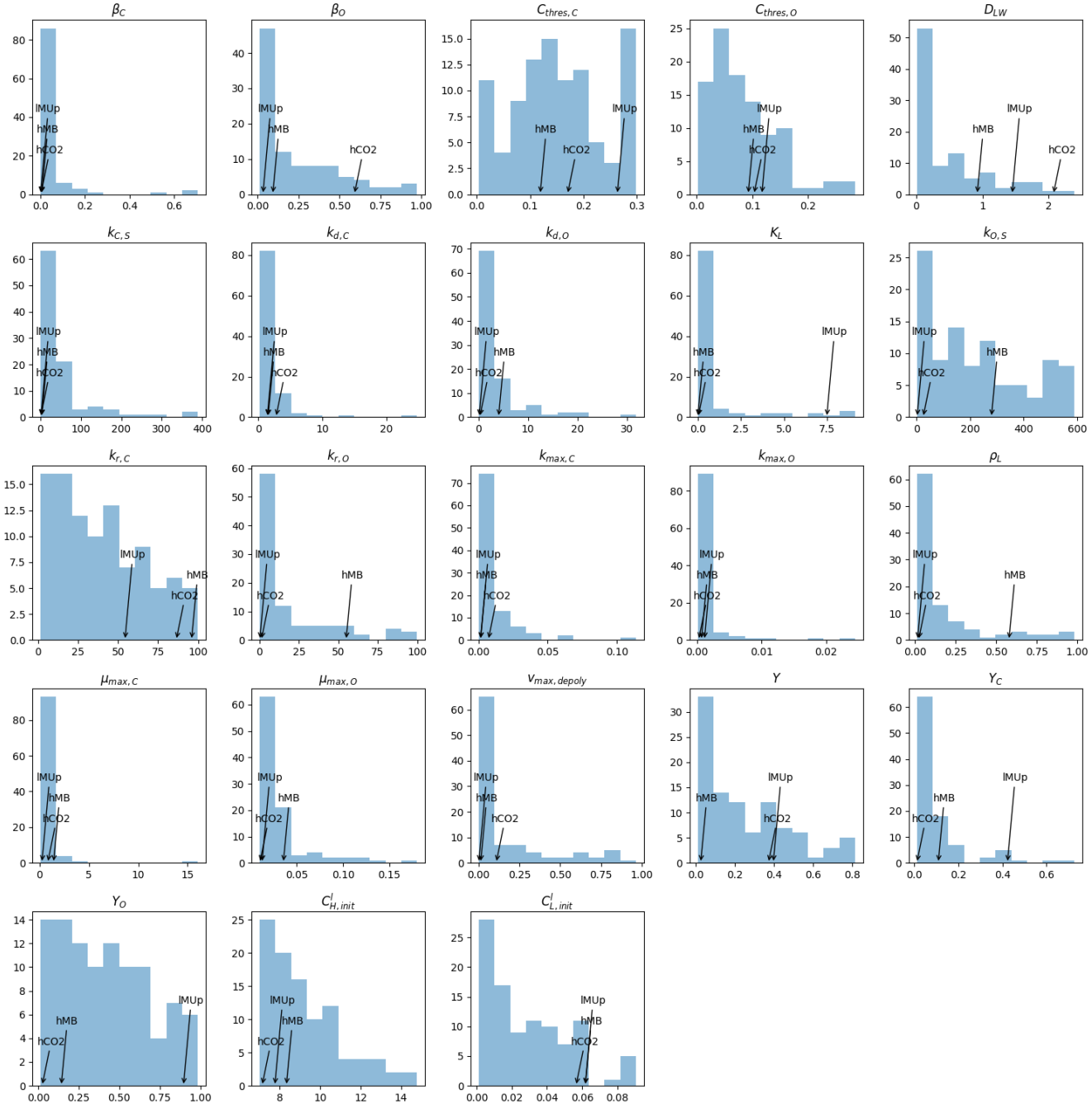


**Figure I2. Histogram of the TraiRhizo input parameters**. The parameters pointed by the numbered arrows correspond to the parameters of the three selected sets, *highCO2*, *highMB*, *lowMUptake*, respectively called *hCO2*, *hMB*, *lMUp*.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


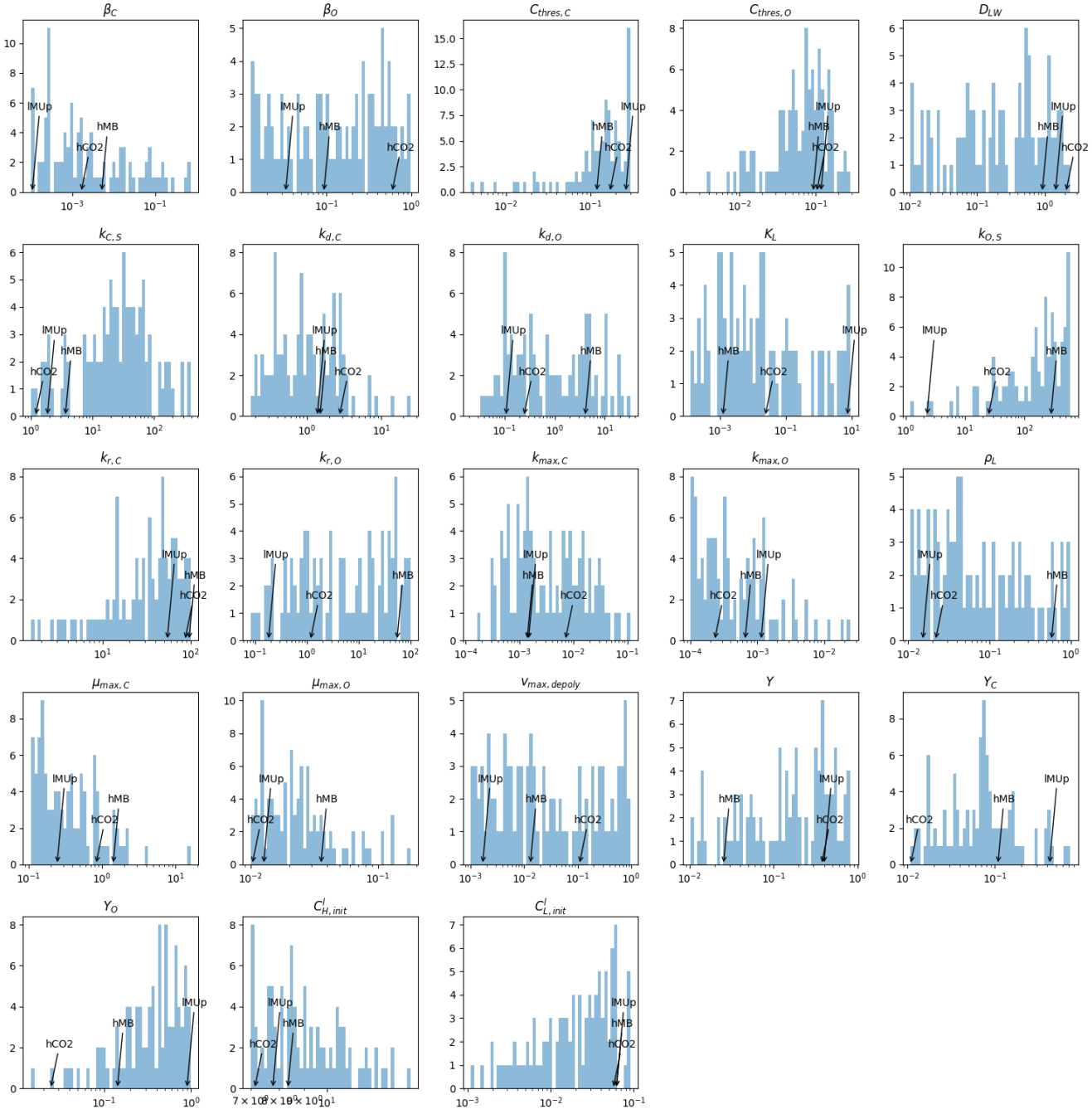


**Figure I3. Logarithmic histogram of the TraiRhizo input parameters**. he parameters pointed by the numbered arrows correspond to the parameters of the three selected sets, *highCO2*, *highMB*, *lowMUptake*, respectively called *hCO2*, *hMB*, *lMUp*.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


### I2.2 Distribution of output variables under different values of dissolved low molecular weight organic carbon

We computed for a range of $C_L^l$ values intermediary outputs describing the microbial dynamic:

- $\phi_O$ ($\phi_C$), $-$: ratio of oligotrophs (copiotrophs) which will be activated
- $S_{decay}$, $mol\ C\ cm^{-3}\ d^{-1}$: decay rate
- $S_{growth}$, $mol\ C\ cm^{-3}\ d^{-1}$: growth rate
- $S_{deact}$, $mol\ C\ cm^{-3}\ d^{-1}$: deactivation rate of active microbes
- $S_{react}$, $mol\ C\ cm^{-3}\ d^{-1}$: reactivation rate of dormant microbes
- $dCO2dt$, $mol\ C\ cm^{-3}\ d^{-1}$: production rate of CO2
- $dMBdt$, $mol\ C\ cm^{-3}\ d^{-1}$: total absolute amount of change in the mass of microbial biomass C per unit of time

Fig.I4 give the ratio between the related intermediary variables for all the parameter sets with the selected sets being colored. Fig. I5 shows the same data but only for the selected sets. Subgraphics d to i use a logarithmic scale on the y-axis. As we can observe, *highCO2* led to a higher relative advantage of the oligotroph compared with the copiotroph regarding their fitness (decay-to-growth rate ratio). This was driven by the higher copiotroph decay-to-growth rate ratio. This was partly compensated by the lower ratio $\frac{S_{growthC}+S_{decayC}}{S_{deactC}+S_{reactC}}$ indicating that the copiotroph dynamic was more driven by (de)activation than by growth and decay. Moreover, we can note a higher $CO_2$ emission rate per unit of transformed microbial C.

*highMB* had lower $\phi$ values for both copiotrophs and oligotrophs, indicating that lower $C_L^l$ values was necessary for an activation of the microbial community. This led in part to the lower $\frac{S_{deact}}{S_{react}}$ for both microbial group, causing a quicker reactivation compared with the deactivation. *highMB* also led to relatively low decay-to-growth ratio when compared with the other two sets. Finally, for lower $C_L^l$ values, *highMB* had the highest relative importance of (de)activation on the copiotroph dynamic, when compared with the other two sets. *lowMUptake* offered the highest copiotroph fitness and the lowest oligotroph-to-copiotroph fitness ratio, giving a relative advantage to the copiotrophs. However, this set had the highest $\phi$ and $\frac{S_{deact}}{S_{react}}$ values, leading to a stronger deactivation of the microbes. For this set, we have a higher importance of the growth and decay over the (de)activation when comparing with the other two sets.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


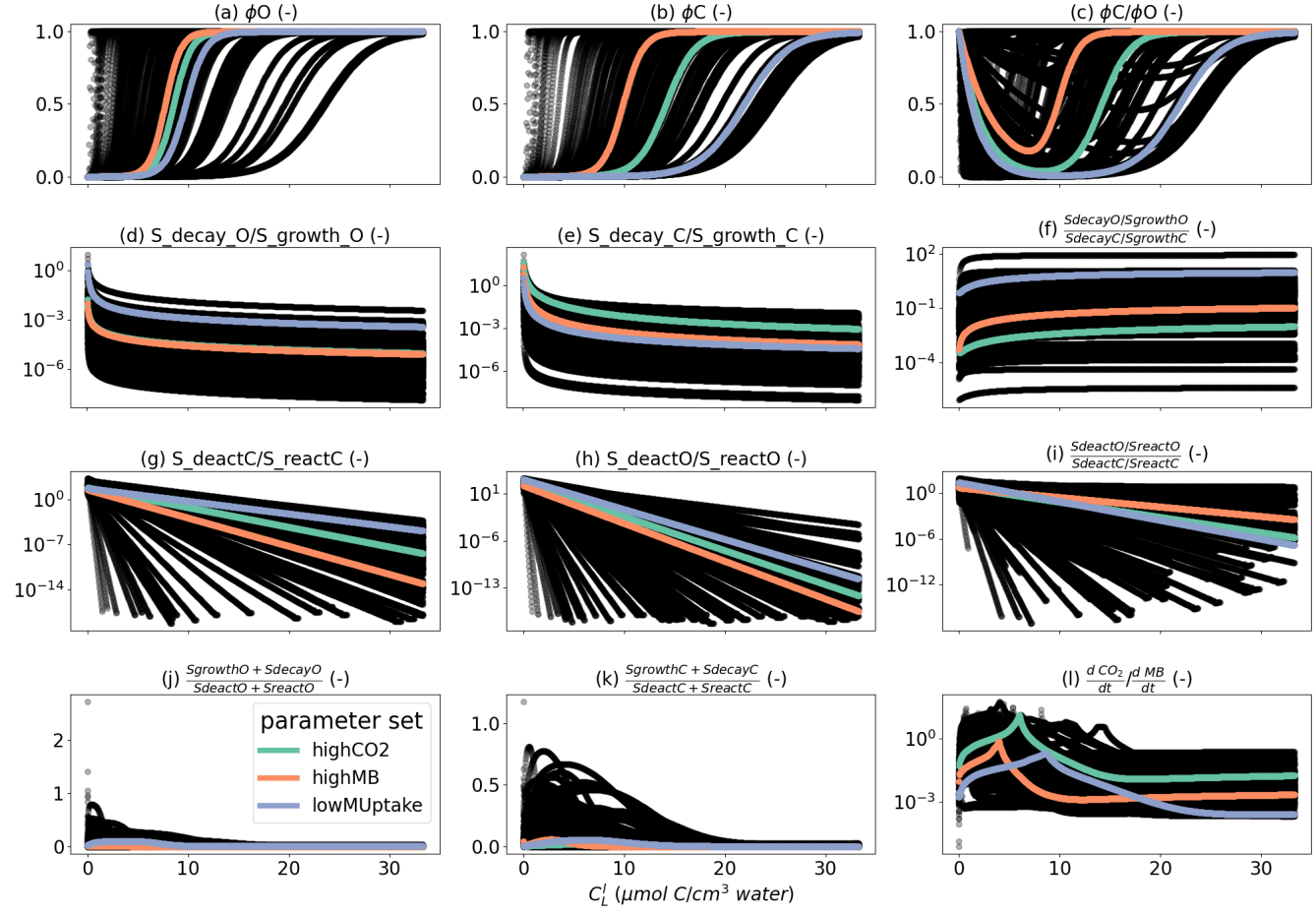


**Figure I4. Distribution of specific microbial-related reaction rate for a range of $C_L^l$ for all 99 parameter sets**. The coloured values correspond to the three selected sets: *highCO2* (green line), *highMB* (orange line) and *lowMUptake* (purple line). Graphics d to i use a logarithmic scale for the y-axis.

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


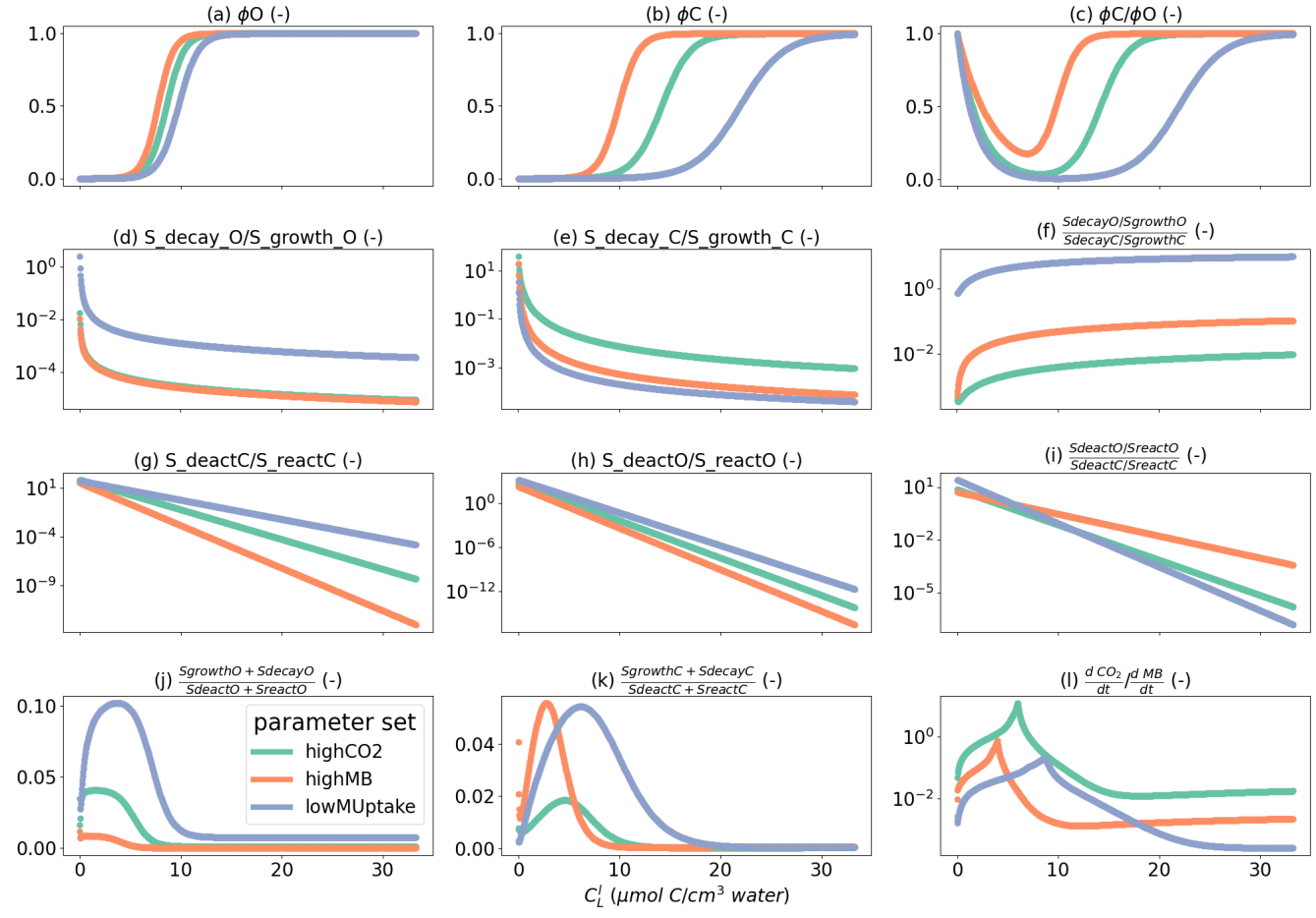


**Figure I5. Distribution of specific microbial-related reaction rate for a range of $C_L^l$ for the selected parameter sets**. The coloured values correspond to the three selected sets: *highCO2* (green line), *highMB* (orange line) and *lowMUptake* (purple line). Graphics d to i use a logarithmic scale for the y-axis.

## Appendix J: Complementary results

### J1 Model runtime

The model was implemented on the Institute of Bio- and Geosciences (IBG-3) computer cluster, Forschungszentrum Jülich. Each simulation was run on one node (shared memory) and 32 cores (Mainboard Supermicro H12DSU-iN), using all 32 cores for the simulation of the 1D and 3D soil domains (respectively the micro- and macroscale) and one core for the plant domain. The run-time of the simulation lasted between 9 $h$ (*baseline* with *highSolutes*) and 13 $h$ (*lateDry* with *highCO2*). The time step of the fixed point iteration remained at 20 $mn$ for the baseline scenarios, went several times down to 7 $mn$ for the *earlyDry* and *lateDry* scenarios. The computation of the water flows and content was the main bottleneck for the convergence of the

https://doi.org/10.5194/egusphere-2025-572
Preprint. Discussion started: 7 March 2025


iteration loop. For *baseline*, respectively 17%, 10%, and 27% of the runtime was spent solving the 3D soil domain, 1D soil domain, and plant models. For *earlyDry*, on average, 36%, 9%, and 14% of the runtime was spent solving the 3D soil domain, 1D soil domains, and plant models. For *lateDry*, on average, 38%, 11%, and 15% of the runtime is spent solving the 3D soil domain, 1D soil domain, and plant model. In total, between 54% and 64% of the runtime was dedicated to solving the models.

### J2 Normalised root length density

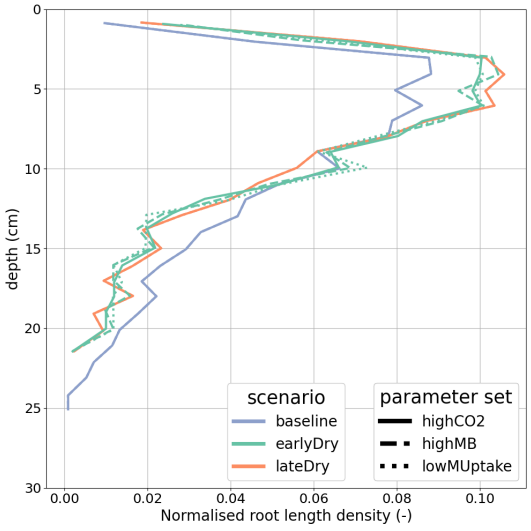


**Figure J1. Normalised root length density** at the end of the simulation. Line colours indicate the weather scenarios: baseline (blue) against an early (green) and late (red) dry spell. Line types represent different biokinetic parameter sets.

## Appendix K: Radial carbon concentration profiles

To evaluate how $C_L^l$ is linked with the development and activation of the most important microbial pool (copiotrophs), Fig. K1 presents the radial concentration profile of the $C_C$ and $C_C^a$:$C_C$ ratio at the end of the simulations. We observed a very steep gradient of $C_C$ according to the distance from the root surface for *highMB* and *highCO2*. Indeed, the microbes developed around the C source. As they were not motile, they remained on this segment even once the root segment had become older and its C releases and water uptake decreased. For *lowMUptake*, the $C_C$ gradient (like the $C_l^l$ gradient, see Fig. 12) was smoother than the other two parameter sets for all weather scenarios. Therefore, even though $C_C$ directly at the root-soil interface is higher with *highCO2* than with *lowMUptake*, we observed similar $C_C$ at the bulk soil and perirhizal$_{trunc}$ scales (Figs. 8(e) and 9(d)).

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Preprint. Discussion started: 7 March 2025


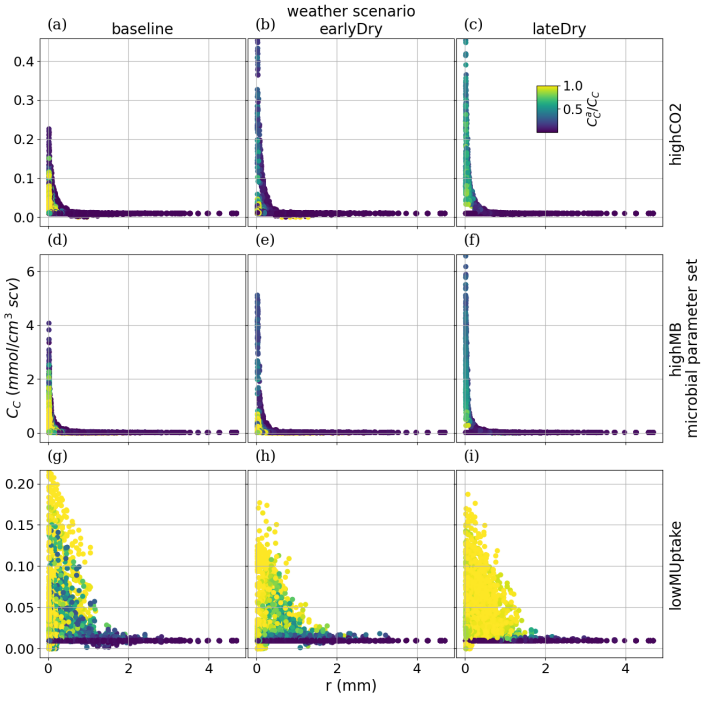


**Figure K1. radial concentration profile of copiotroph carbon** at the end of the simulation for each plant perirhizal zone. $r$ $(mm)$ corresponds to the distance to the root surface. The colour gives the ratio of active-to-total oligotroph biomass. Each column corresponds to a specific weather scenario and each row corresponds to a specific biokinetic parameterisation. We have a different y-axis for each row.

## . Author contribution

MG: Development and implementation of the new modules, Output visualization, Writing – original draft, Writing – review and editing. AKS: Definition of the parameter space. MG, AKS: Setup of the equation set, Output analysis, Writing – review and editing. AS, GL, HP, TS: Output analysis, Setup equation set, Writing – review and editing, Setup of the project and Funding acquisition, Supervision. GL, AS, HP: Support with the model development. MG and AKS contributed equally to the study. AS and HG supervised equally this study.

## . Competing interests

The authors declare that they have no conflict of interest.

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