

Original Article

CPlantBox: a fully coupled modelling platform for the water and carbon fluxes in the soil–plant–atmosphere continuum

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ABSTRACT

A plant's development is strongly linked to the water and carbon flows in the soil–plant–atmosphere continuum. Expected climate shifts will alter the water and carbon cycles and will affect plant phenotypes. Comprehensive models that simulate mechanistically and dynamically the feedback loops between a plant's three-dimensional development and the water and carbon flows are useful tools to evaluate the sustainability of genotype–environment–management combinations which do not yet exist. In this study, we present the latest version of the open-source three-dimensional Functional–Structural Plant Model CPlantBox with P1afMunch and DuMu^x coupling. This new implementation can be used to study the interactions between known or hypothetical processes at the plant scale. We simulated semi-mechanistically the development of generic C3 monocots from 10 to 25 days after sowing and undergoing an atmospheric dry spell of 1 week (no precipitation). We compared the results for dry spells starting on different days (Day 11 or 18) against a wetter and colder baseline scenario. Compared with the baseline, the dry spells led to a lower instantaneous water-use efficiency. Moreover, the temperature-induced increased enzymatic activity led to a higher maintenance respiration which diminished the amount of sucrose available for growth. Both of these effects were stronger for the later dry spell compared with the early dry spell. We could thus use CPlantBox to simulate diverging emerging processes (like carbon partitioning) defining the plants' phenotypic plasticity response to their environment. The model remains to be validated against independent observations of the soil–plant–atmosphere continuum.

KEYWORDS: CPlantBox; functional–structural plant model; genotype-by-environment-by-management interactions; phenotypic plasticity; plant modelling; soil–plant–atmosphere continuum

1. INTRODUCTION

Terrestrial carbon and water cycles are, amongst others, affected by plant development (De Swaef et al. 2022; De Schepper et al. 2013; Vries 2021). Climate change is expected to alter the global water and carbon balances (Swart et al. 2019) and thus plant phenotype and fitness (Vries 2021). A better understanding of the mechanisms driving the plant carbon and water fluxes, and their relations to the environment is key to selecting phenotypes

and management practices, which are adapted to these altered environmental conditions and therefore to mitigate the negative effects of climate change and maintain or even increase food production (De Swaef et al. 2022; Galindo-Castañeda et al. 2022; Soualiou et al. 2021; Vries 2021).

However, the complex spatio-temporal interactions between the water and carbon fluxes in the soil–plant–atmosphere continuum make predictions and analyses of experimental results

difficult. First of all, cellular scale characteristics (like the shape and size of the xylem and phloem tissues) need to be considered to understand emerging effects seen at larger scale (like the evapotranspiration and biomass production of a field) (Cabrita 2011; Bramley 2006; M. Thompson and N. Holbrook 2003; Coussement et al. 2020). Moreover, feedback loops and threshold effects make the influence of plant physiological traits on the water and carbon cycles site specific (Vries 2021). For these same reasons, we can also observe differences between short- and long-term effects of climatic shifts on the water and carbon cycles (Damour et al. 2010; Vries 2021) and experimental studies are not sufficient to predict the equilibrium of ecosystems in the distant future.

Mechanistic modelling can help evaluate plant behaviour for as yet non-existing genotype–environment–management combinations and can help decipher underlying interrelated processes leading to experimental observations (Stanfield and Bartlett 2022; Tuzet, Perrier, and Leuning 2003; Soualiou et al. 2021). Modelling can, therefore, be used to investigate the benefits and drawbacks of novel crop management practices and to set objectives for plant breeders (Stanfield and Bartlett 2022; Louarn and Song 2020; Soualiou et al. 2021).

From three-dimensional functional–structural plant model (3D FSPMs) properties emerge at the organism scale that can be scaled up to the field or ecosystem (De Swaef et al. 2022; Louarn and Song 2020; Soualiou et al. 2021). Functional–structural plant models that represent the transport functions of plant tissues are especially adapted to simulate plant carbon and water fluxes in the plant and link these fluxes to (i) the water and carbon transfer in the environments (soil and atmosphere), (ii) the smaller and larger scale structures of the plant, and (iii) its growth and development (Cannell and J. H. M. Thornley 2000; Lacointe and Peter E. H. Minchin 2019; Coussement et al. 2020). For instance, axial flow (along the transport tissues) can be represented by Darcy's law. Likewise, lateral flow (leaving or entering the transport tissues), which involves transport across selective plant cell membranes, can be represented by a membrane transport equation (Meunier et al. 2017; M. Thompson and N. Holbrook 2003; Zhou et al. 2020) and depends on pressure or osmotic potential gradients. The plant water and carbon fluxes are hence the results of (i) cellular-scale characteristics, like the number of cell layers between the vascular bundles and the epidermis (Bramley 2006); (ii) plant-scale characteristics, like the topology of the xylem and phloem networks (Lacointe and Peter E. H. Minchin 2019); and (iii) water potentials in the soil and atmosphere and photosynthesis and local sink terms that determine sugar concentrations in the phloem. Therefore, FSPMs with transport functions should be able to predict the fluxes of carbohydrates and water from sources to sinks and determine organ growth as a function of plant-external conditions. This implies that these FSPMs should be able to reproduce phenotypic plasticity in different climates and could complement crop models by supplying plant structure parameters, like the ratio of shoot-to-root biomass, computed semi-mechanistically under specific genotype–environment–management combinations.

The quality and applicability of an FSPM depend on the processes and domains it considers: linking different mechanisms (like the flow and use of carbon), domains (soil, plant and

atmosphere) and organs (root, shoot, etc.) via dynamic feedback loops is essential to understand the short- to long-term effects of specific plant traits on the plant capacity to adapt to the environment (Tuzet, Perrier, and Leuning 2003; Louarn and Song 2020). For instance, the short feedback loop between the plant stomatal regulation, water and carbon flows needs to be represented. Indeed, the photosynthesis (source of plant carbon) and transpiration (loss of plant water) occur through the same path and are both influenced by the stomatal opening (Corso et al. 2020; Damour et al. 2010; Dewar 2002). This loss of water (resp. source of carbon) is interlinked with the xylem (resp. phloem) turgor pressure gradients that drive the flow in the transport tissues (M. Thompson and N. Holbrook 2003). As the stomatal opening also depends on the leaf water status, it is itself influenced by the flow of water in the xylem (Damour et al. 2010; Dewar 2002; Tuzet, Perrier, and Leuning 2003). An important longer-term feedback loop involves the plant growth: carbon and water flows regulate the partitioning of assimilated carbohydrates between the different organs (and resulting shoot-to-root ratio) (De Swaef et al. 2022; Lacointe and Peter E. H. Minchin 2019). The growth will, in turn, indirectly influence the water and carbon fluxes in the soil–plant–atmosphere continuum by changing plant transport network topology and morphology (like the number of roots, leaf area, etc.) and with this, its photosynthetic and water uptake capacities (Damour et al. 2010; Chen et al. 2020; Galindo-Castañeda et al. 2022).

In this work, we present the latest implementation of CPlantBox, a 3D FSPM (Zhou et al. 2020), with PiafMunch (Lacointe and Peter E. H. Minchin 2019) and DuMu^x (Koch et al. 2021) coupling. The novel aspect of this CPlantBox implementation lies in the tight coupling with PiafMunch's carbon flow module, in the implementation of CRootBox modules (like plant growth) (Schnepf et al. 2018) and in the addition of new modules, such as the coupled photosynthesis–transpiration–stomatal regulation (Tuzet, Perrier, and Leuning 2003; Bonan 2019) and water and carbon limitations on growth (De Swaef et al. 2022; Schopfer 2006). While the earlier version of CPlantBox could simulate the effect of a static plant, soil and user-defined transpiration rate on the plant water and carbon fluxes, the new model can also simulate the influence of the plant water and carbon fluxes on the soil water flow, the plant growth and the stomatal regulation. The model can consequently represent semi-mechanistically the interactions between the growth of a 3D plant (discrete structure) and the water and carbon fluxes in the soil–plant–atmosphere continuum (continuum equations). CPlantBox offers thus a generic and precise (high spatial and temporal resolution) framework that can be used to test the interaction between known or hypothetical processes (dynamic of plant carbon and water uptake, flow and usage), and understand the causes of emergent behaviours (exudation rate, carbon partitioning). This new development of the model aims to be user friendly and adapted to a wide variety of plant types. In this paper, we present:

1. An overview of the equations implemented in the new version of CPlantBox and the schemes used to solve them.
2. An application of the model for a generic C3 monocot. The parameters were set using experimental, literature and illustrative data. The model was then implemented to look

at the effect on the plant's development of a dry spell of 1 week at different plant development stages.

2. MATERIAL OF METHODS

2.1. Description of the model

Figure 1 gives an overview of the different processes simulated in CPlantBox. In summary: CPlantBox aims to represent the soil–plant–atmosphere continuum and the interactions between those three domains. The environmental conditions are represented by atmospheric forcing (Fig. 1A.1) and by the soil water initial conditions. The soil water flow equations are then computed during the simulation via the the open-source simulation framework DuMu^x (Koch et al. 2021) (Fig. 1A.3, see Section 2.1.5). The plant domain is represented by a discrete structure made of nodes linked by segments (Fig. 1A.2a, see Section 2.1.2). The atmospheric, leaf boundary layer and soil variables affect the stomatal opening, which regulates transpiration (water sink) and photosynthesis (sucrose source) (Fig. 1A.4, see Section 2.1.4 and Appendix C.3). CPlantBox simulates the resulting xylem water flow, lateral root (and leaf) fluxes and soil–root water exchanges (Fig. 1A.6, see Section 2.1.4). CPlantBox simulates likewise the resulting mesophyll and sieve tube sucrose flow (Fig. 1A.5, see Section 2.1.4). The sucrose dynamic is also influenced by the sucrose usage (or sink), which yields the plant water- and carbon-limited growth, respiration (linked to maintenance and growth) and sucrose exudation (Fig. 1A.7, see Section 2.1.4).

The CPlantBox modules have the following dependency order: plant growth < plant water flow < photosynthesis–stomatal regulation < plant sucrose balance. Therefore, it is possible for the user to run only the lower-level modules (e.g. plant growth and water flow). Likewise, the user can choose whether or not to run the dynamic soil water flow module.

The main differences between the CPlantBox version presented by Zhou et al. (2020) and the current version are presented in section 2.1.1.

In the following sections, we define how plants are represented as a discrete structure in the model (Section 2.1.2). Following this, the equations of the implemented modules are listed (Sections 2.1.2–2.1.5). Finally, we describe the computation loop (Section 2.1.6). The schemes used to solve these continuum models on the discrete plant structures are presented in Appendix F and a sensitivity analysis of the water-related modules and carbon-related modules are presented in Appendix G. A definition of the water potential components and of the conductance or conductivity variables used in this paper as well as their notations are given in Appendix A. Tables presenting the lists of symbols used with their respective units and (when applicable) values can be found in Tables S1–S5 and Table A1.

2.1.1. Comparison with the former CPlantBox implementation

The functional–structural plant model CPlantBox was first presented by Zhou et al. (2020). The differences between the version of Zhou et al. (2020) and the current version of the model are presented in Fig. 2.

In summary, the following modules were added or adapted compared with the original model: (i) the plant meristems can be intercalary, as opposed to apical only (see Section 2.1.3); (ii) water- and carbon-limited growth were implemented (see Section 2.1.4); (iii) the pre-existing xylem water flux analytical solver (Meunier et al. 2017) was expanded from the root to the whole plant and implemented (see Section 2.1.4); (iv) the implicit numerical solver PiafMunch (Lacointe and Peter E. H. Minchin 2019) for phloem flows driven by hydrostatic pressure gradients was adapted for tight coupling to CPlantBox (see Section 2.1.4); (v) the DuMu^x PDE solver (Koch et al. 2021) simulating soil water fluxes with a cell-centred finite volume method (see Section 2.1.5); and (vi) a coupled photosynthesis (FvCB)–stomatal opening (Tuzet, Perrier, and Leuning 2003) was added (see Section 2.1.4).

The tighter coupling between CPlantBox and PiafMunch leads to a higher computation speed and simpler implementation for the end user. Moreover, the changes done to the PiafMunch code allow its implementation with a dynamic (growing) plant.

2.1.2. Structure of the plant

Figure 3A.1 presents a conceptual plant, which is defined as an ensemble of organs. We consider the organs: ‘seed’, ‘root’, ‘stem’ or ‘leaf’. The organ class could be extended to include also other organ categories like, for instance, flowers or fruits. The shape variables are defined with subscripts: *seed*, *root*, *stem*, *leaf*, *st* (sieve tube tissues), *x* (xylem tissues), *seg* (segment), *org* (organ), *sheath* (leaf sheath) or *blade* (leaf blade).

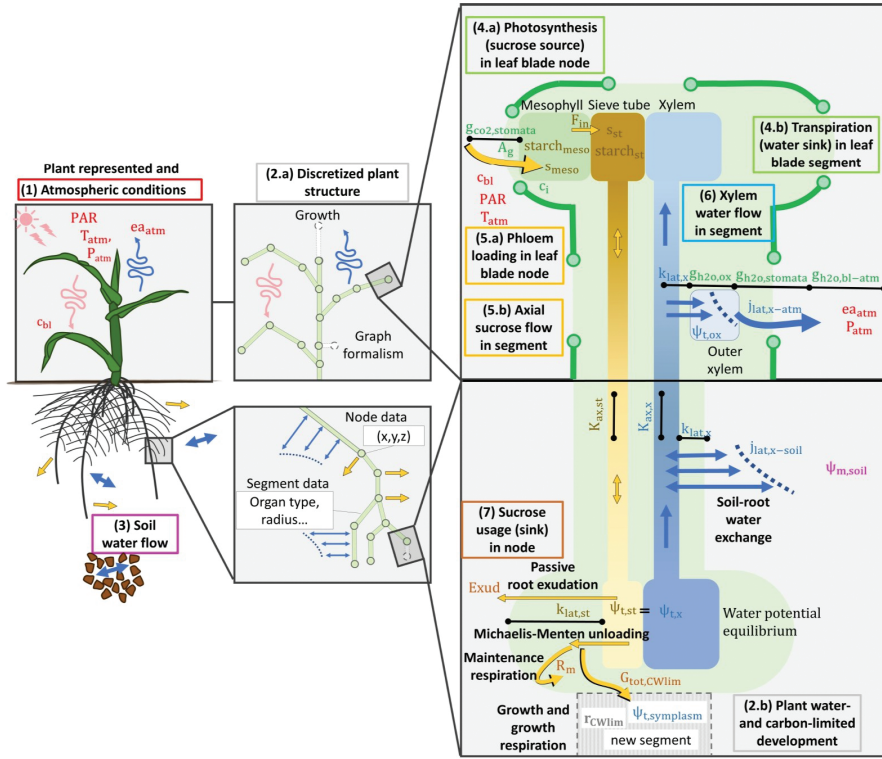
As represented in Figs. 1A.2a and 3B, plant organs are seen as a series of cylinders (root or stem segments) or cuboids (leaf segments).

As shown in Fig. 3C, the conceptual plant topology is represented in a discrete way in CPlantBox using graph formalism: the organs are made of 1D segments, which are defined by their begin and end nodes (directed tree). Each node has 3D coordinates. The orientation of the segments has an effect on the sign of the inner plant flows Appendix F.1. CPlantBox stores one mean value per segment of each variable defining the plant's morphology, like cylinder radius (or cuboid thickness) a , and cuboid width w , both in centimetres. Although the sieve tubes and xylem tissues are not explicitly represented, their data are also stored, for instance: number of xylem vessels per cross section (n_x) and radius (a_x). This allows us to directly use or compute at run time the necessary plant variables.

More information regarding the plant conceptual shape and the related equations can be found in Appendix B.

The plant growth rate can either follow an empirical function or, when the water and sucrose modules are run, the water- and sucrose-limited growth rate (r_{CWlim} in cm day^{-1}), can be used (Fig. 1A.2b). The equations used to compute r_{CWlim} are presented in Appendix 2.1.3. In brief, the initial potential (maximum) organ growth rate is user defined. CPlantBox then computes the current potential organ growth rate, the limitation caused by the symplast turgor pressure ($\psi_{p,symplast}$ in hPa) and by the supply of sucrose. This yields r_{CWlim} , the actual growth

(A) **graphical overview.** The water content and flow are defined along the segments. The sucrose concentration and sink or source rates are defined for each plant node. Growth-related sinks can occur in all meristem nodes, maintenance can occur in all nodes, and exudation can occur in all root nodes. Assimilation can occur in all leaf-blade nodes.



(3) Soil water flow

$$\frac{\partial \theta_{soil}}{\partial t} - \nabla \cdot (\kappa_{soil}(\theta_{soil})(\nabla \psi_{m,soil} + \nabla \psi_g)) = \frac{1}{V_{soil}} \sum_{i=1}^N (\text{Surface}_i \times j_{lat,x-soil}), \text{ Eqn.(51)}$$

$$\theta_{soil}(\psi_{m,soil}) = \theta_{r,soil} + \frac{\theta_{s,soil} - \theta_{r,soil}}{[1 + (-\alpha_{soil} \psi_{m,soil})^n]^{1-1/n}}, \text{ Eqn.(52)}$$

$$\kappa_{soil}(\theta_{soil}) =$$

$$\kappa_{soil}(\theta_{soil}) \frac{(1 - (\alpha_{soil} |\psi_{m,soil}|)^{n_{soil}})^{n_{soil}-1} [1 + (\alpha_{soil} |\psi_{m,soil}|)^{n_{soil}}]^{n_{soil}}}{[1 + (\alpha_{soil} |\psi_{m,soil}|)^{n_{soil}}]^{n_{soil}/2}}.$$

$$\text{Eqn.(54)}$$

(4) Stomatal regulation, photosynthesis and transpiration

$$j_{lat,ox-atm} = \frac{M_{h2o}}{\rho_{h2o}} g_{h2o,ox-atm} \frac{ea_{ox} - ea_{atm}}{P_{atm}}, \text{ Eqn.(2)}$$

$$\psi_{p,ox} = \psi_{p,x} - \frac{j_{lat,x-atm}}{k_{lat,x}}, \text{ Eqn.(3)}$$

$$A_n = \min(F_c(T_{atm}), F_j(T_{atm}, PAR)) - R_d, \text{ Eqn.(13-14)}$$

$$g_{co2,stomata} = (g_{0,co2,stomata} + \frac{k_{g1} A_n}{c_i - \Gamma}) \times f_{w1}(\psi_{p,ox}), \text{ Eqn.(18)}$$

$$c_i = \frac{c_{bl} k_{g1} f_{w1}(\psi_{p,ox}) + \Gamma}{1 + k_{g1} f_{w1}(\psi_{p,ox})}, \text{ Eqn.(22)}$$

(5) Plant sucrose flow

$$\frac{\partial s_{st}}{\partial t} + \frac{\partial}{\partial \xi} \left(s_{st} \times K_{ax,st} \left(RT \frac{\partial s_{st}}{\partial \xi} + \frac{\partial \psi_{t,x}}{\partial \xi} \right) \right) =$$

$$F_{in}(s_{meso}) - F_{out} - \frac{\partial \text{starch}_{st}}{\partial t},$$

$$\text{for } \Omega, \text{ Eqn.(34)}$$

$$K_{ax,st} \left(RT \frac{\partial s_{st}}{\partial \xi} + \frac{\partial \psi_{t,x}}{\partial \xi} \right) = 0 \text{ for } \partial \Omega. \text{ Eqn.(36)}$$

$$\frac{\partial s_{meso}}{\partial t} = \frac{A_g \text{ Surface}_{blade}}{12 \text{ Vol}_{meso}} - \frac{\partial \text{starch}_{meso}}{\partial t} - F_{in}, \text{ Eqn.(37)}$$

(6) Xylem water flow

$$j_{lat,x-out} = \begin{cases} j_{lat,x-atm} = k_{r,x}(\psi_{p,x} - \psi_{p,ox}), \\ j_{lat,x-soil} = k_{r,x}(\psi_{p,x} - \psi_{m,soil}), \end{cases} \text{ Eqn.(26)}$$

$$-K_{ax,x} \frac{\partial^2 \psi_{p,x}}{\partial \xi^2} = -\text{Perimeter} \times j_{lat,x-out}, \text{ for } \Omega, \text{ Eqn.(27)}$$

$$\frac{\partial \psi_{t,x}}{\partial \xi} = 0 \text{ for } \partial \Omega. \text{ Eqn.(28)}$$

(7) Sucrose usage

$$[F_{out,MM}] = ([R_{m,max}] + [Gr_{tot,Wlim}(\psi_{t,x})]) \frac{s_{st}}{s_{st} + M_{out}}. \text{ Eqn.(47)}$$

$$[F_{out}] = [F_{out,MM}] + [Exud], \text{ Eqn.(48)}$$

Figure 1. Representation of the domains and processes simulated within CPlantBox.

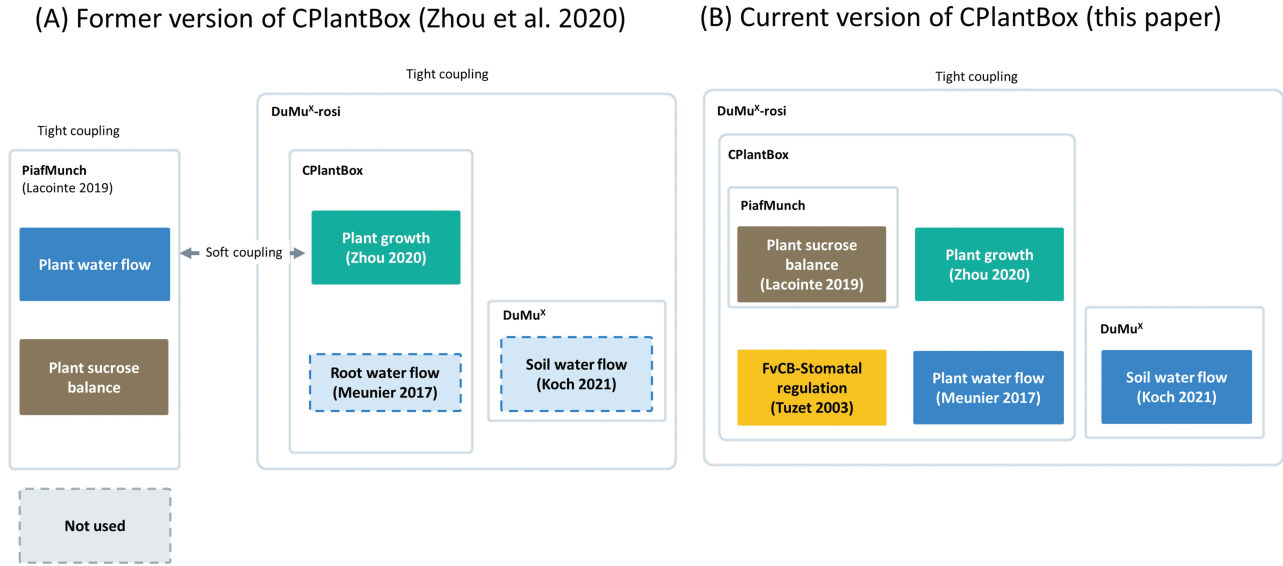


Figure 2. Evolution of CPlantBox within the DuMuX-ROSI interaction framework. Representation of (A) the former and (B) current versions of CPlantBox. The main changes include an expansion of the root water flow module to shoot organs, implementation of a photosynthesis (FvCB) and stomatal opening module, and adaptation and implementation within CPlantBox of a phloem flow module. The tighter coupling between the phloem and plant module allows us to use the CPlantBox water module and the DuMuX soil flow module.

rate. This growth is represented via the elongation of existing segments or via the creation of new segments.

The lateral growth of the xylem and phloem tissues can be represented by setting a time-dependent axial conductance, lateral conductivity as well as a time-dependent cross-sectional area of the phloem vessels ($A_{\text{cross},st}$ in cm^2). We neglect the elastic (reversible) variation of the tissue volumes (v in cm^3) according to the turgor pressures (ψ_p in hPa).

The explicit representation of the plant segment and their growth in CPlantBox is presented in more detail by Schnepf et al. (2018).

2.1.3. Maximum and carbon- and water-limited growth rate

$r_{\text{max,org}}$ ($\text{cm}^3 \text{ day}^{-1}$) is the maximum irreversible growth rate of the organ's growing zone when the cell's symplast is at full turgor and the xylem is at the reference water potential ($\psi_{t,x} = 0$). To compute the carbon need for growth ($G_{\text{tot,max}}$, $\text{mmol sucrose day}^{-1}$), we first divide this growth demand between the nodes of the segments within the growing zone (using the dimensionless f_{length} factor). The water-limited growth rate ($r_{\text{Wlim},i}$ in $\text{cm}^3 \text{ day}^{-1}$) and carbon need ($G_{\text{tot,Wlim}}$, $\text{mmol sucrose day}^{-1}$) are computed for the node i as follows:

$$r_{\text{Wlim},i} = r_{\text{max,org}} \times f_{w2} \times f_{\text{length}} \quad (1)$$

$$f_{w2} = \frac{\max(\psi_{p,\text{symplast}}, \psi_{p,\text{crit},2}) - \psi_{p,\text{crit},2}}{-\psi_{o,\text{symplast}} - \psi_{p,\text{crit},2}} \quad (2)$$

$$r_{\text{max,org}} = \frac{v_{\text{end,org}} - v_{\text{init,org}}}{t_{\text{end}} - t_{\text{init}}} + \frac{v_{\text{end,org,child}} - v_{\text{init,org,child}}}{t_{\text{end}} - t_{\text{init}}} \quad (3)$$

$\psi_{p,\text{symplast}}$ (cm) is the turgor water pressure within the symplast of the cell. $\psi_{p,\text{crit},2}$ is the minimum symplast turgor potential

below which no growth occurs (the 'wall yield threshold'). We assume that the apoplast has the same water potential values as the xylem tissues and that the permeability of the membrane between the apoplast and the symplast is high: $\psi_{t,\text{apoplast}} = \psi_{t,x}$ (De Swaef et al. 2022; Schopfer 2006). We thus obtain $\psi_{p,\text{symplast}} = \psi_{t,x} - \psi_{o,\text{symplast}}$. Also, we do not represent the osmotic regulation to drought. Therefore, we consider that the osmotic water potential in the symplast $\psi_{o,\text{symplast}}$ is constant. f_{w2} increases consequently linearly with $\psi_{t,x}$.

As we neglect the elastic flexibility of the cell walls, Equation (2) is conceptually similar to Zubairova et al. (2016, Equation 6). To facilitate the calibration from empirical data, we normalized the gradient between $\psi_{p,\text{symplast}}$ and $\psi_{p,\text{crit},2}$ to obtain the dimensionless f_{w2} , which can be multiplied by $r_{\text{max,org}}$. The variation of $r_{\text{max,org}}$ according to a negative exponential function (Schnepf et al. 2018; Zhou et al. 2020) can be used to represent implicitly the variation of the irreversible wall extensibility.

The volume of the organs according to their length can be computed from the formulas given in Appendix B.

$v_{\text{org,child}}$ corresponds to the volume of the child (lateral) organs attached to the node i and which are too small to be explicitly represented in the plant structure. They, therefore, use the sucrose of parent organ's node they are connected to.

As shown in Fig. 4, the growth zone ($l_{\text{growingZone}}$ in cm) of roots is located at the organs' tip (Bramley 2006), while the leaf-growing zone is within the first centimetres at the base of the leaf (Zubairova et al. 2016). For the stem, the growing zone is within the growing phytomer (Kirby 1988). These growing zones correspond to the organ nodes where $G_{\text{tot,max}} > 0$. Therefore:

$$f_{\text{length}} = \frac{l_{\text{seg} \cap \text{growingZone}}}{l_{\text{growingZone}}} \quad (4)$$

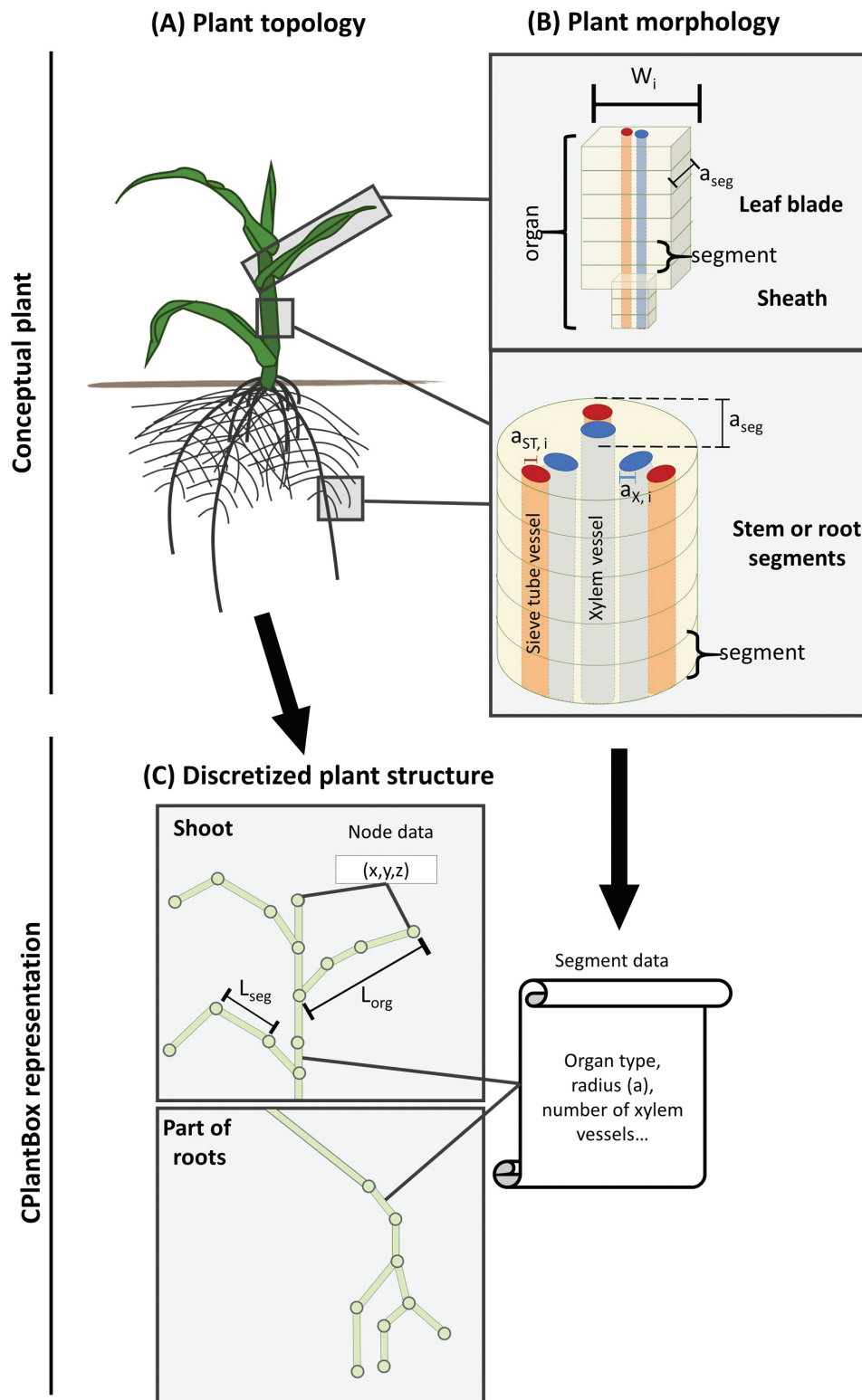


Figure 3. Representation of a conceptual plant's topology (A), the morphology of its organs (B) and its discretized representation in CPlantBox (C). The plant topology is represented by the nodes' 3D coordinates and by their connections (segments). The morphological data are stored in arrays with one value per segment. Note: For better visibility, the cross section of the xylem and phloem vessels is not at the scale of the organs' cross sections.

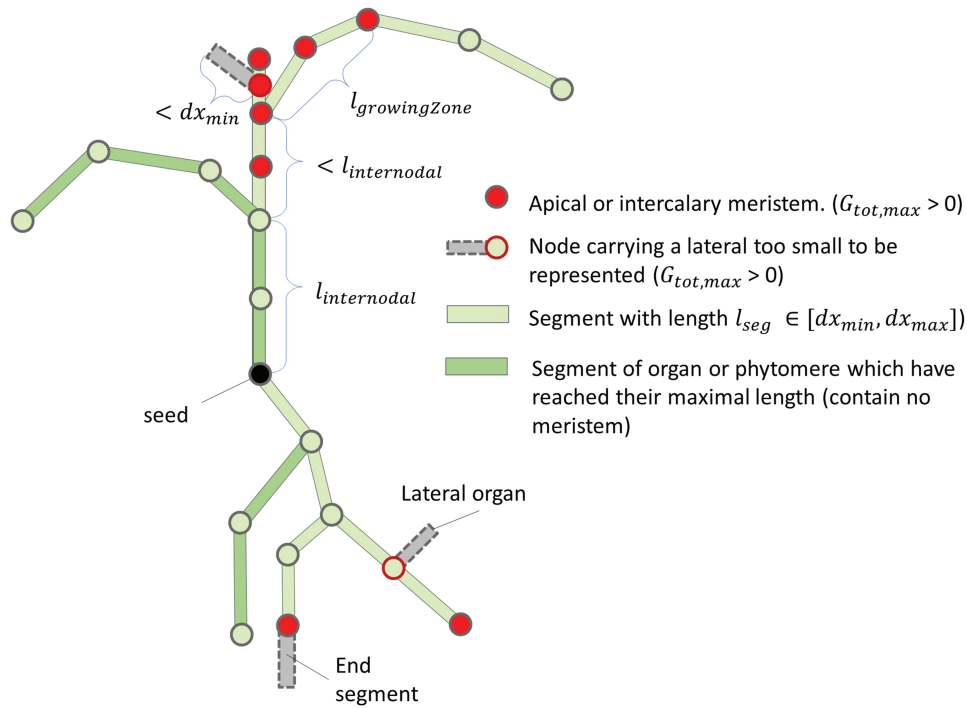


Figure 4. Location of a plant's meristems (red-filled points, first item of the legend). Roots have apical meristem. Leaves have intercalary meristem at their base. Stems with internode elongation have intercalary meristems in each phytomere. These meristem nodes are carbon sinks used in the sucrose flow module. When segments with meristems are too small to be represented ($l_{\text{seg}} < dx_{\text{min}}$), like for small laterals or end segment of organs, the nearest node is used as carbon sink (points with red outline, second item of the legend).

With $l_{\text{seg} \cap \text{growingZone}}$ the part of the segment which is within $l_{\text{growingZone}}$.

After running the phloem module, the water- and carbon-limited growth rates ($r_{\text{CWlim},i}$, $\text{cm}^3 \text{ day}^{-1}$) for the node i are computed as follows:

$$r_{\text{CWlim},i} = \frac{G_{\text{tot,CWlim},i} \times Y}{\rho_s} \quad (5)$$

with ρ_s ($\text{mmol sucrose cm}^{-3}$) the plant tissue sucrose density, Y (–) the efficiency of the plant sucrose usage for growth. $G_{\text{tot},i}$ ($\text{mmol sucrose day}^{-1}$) is the actual (carbon- and water-limited) plant sucrose usage rate for growth and growth-related respiration given by the sucrose module (see Equation (54)). $r_{\text{CWlim},i}$ of the nodes in the growing zone (cell division and cell elongation) will then be used by CPlantBox to simulate the organ growth.

For leaves and stems, this representation creates a small growth compensation (artificial carbon flow) within the organ's growing zone (first centimetres of the leaf or growing phytomere of the stem). For example, carbon used for growth at the start of the growth section can lead to an elongation at the end of the growth section.

A precise description of the methods used in CPlantBox to create segments and define their orientation is presented in Schnepf et al. (2018). In brief, each time a new node is added, the tropism (resp. bending) function is called *TropismN* (resp. *bendingN*) times. Sets of α and β (rad) angles are drawn from, respectively, a normal distribution with zero mean and standard

deviation *TropismS* (resp. *bendingS*, in cm^{-1}) and a uniform distribution between 0 and 2π . The α and β set leading to the optimization of the tropism (resp. bending) function is kept (see Fig. 5.1).

Some functionalities were added in the new version of CPlantBox. It is now possible for existing nodes to be shifted (see Fig. 5.2), elongating thus the length of the prior segment. For intercalary meristems, this leads to the shift of all the subsequent nodes. In such cases, the directions of the following segments are re-computed.

2.1.4. Functions within the plant

Stomatal regulation, photosynthesis, and transpiration In the following section, we present the FvCB-stomatal regulation module (see Fig. 1A.4) (Farquhar, Caemmerer, and Berry 1980; Leuning 1995; Tuzet, Perrier, and Leuning 2003). Transpiration and photosynthesis outside of the leaf blades were neglected. Outputs include (i) the net assimilation rate (A_n in $\text{mmol C cm}^{-2} \text{ day}^{-1}$), which is the source term used by the sucrose flow module (see Equation (41)), and (ii) the leaf outer-xylem water potential ($\psi_{t,ox}$ in hPa), which is used by the xylem module (see Equation (30)).

Leaf transpiration rate and stomatal hydraulic conductivity As presented in Fig. 6, the water vapour has to go through several compartments, defined by their respective conductances $g_{\text{H}_2\text{O},Y}$ ($\text{mmol cm}^{-2} \text{ day}^{-1}$); with Y standing for the outer-xylem pathway to the stomata (ox), the stomata (stomata), the leaf boundary layer (bl), the canopy above the leaf (canopy),

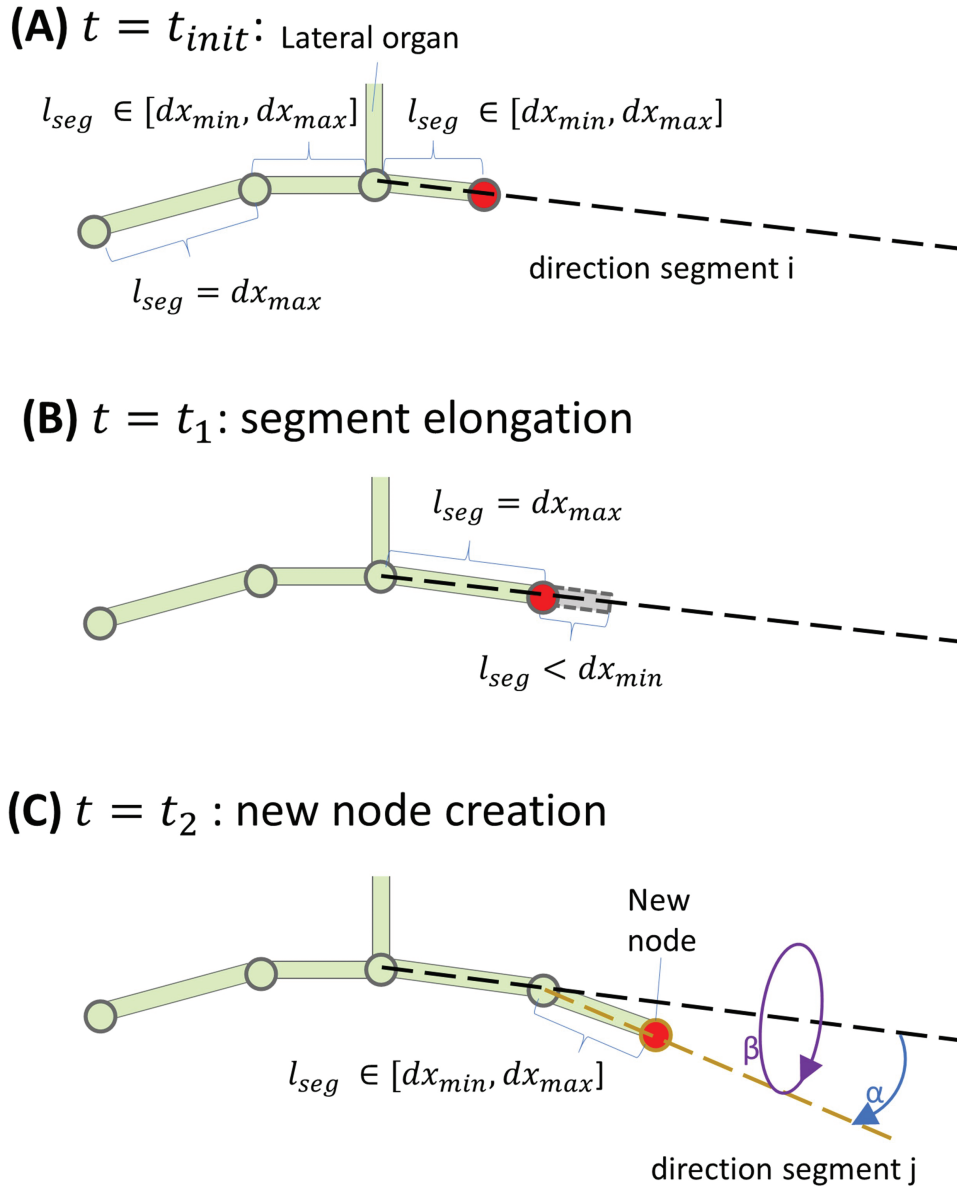


Figure 5. Growth of the discretized plant structure. (A) All segments have a length $l_{seg} > dx_{min}$. (B) All segments are elongated until reaching $l_{seg} = dx_{max}$, unless the internodal distance is reached beforehand. Segments of length $l_{seg} < dx_{min}$ are not represented. (C) Once a segment has reached its maximum length, the organ is further elongated by adding a new node. The position of the new node is selected according to the result of the tropism (roots) or bending (shoot) function. Adapted from Schnepf et al. (2018, Figure A1)

or the air between the top of the canopy and the point of measurement (atm). The total conductance between the outer xylem compartment and the point of humidity measurement ($g_{H_2O,ox-atm}$ in $\text{mmol cm}^{-2} \text{day}^{-1}$) is obtained by analogy with electric resistances in series:

$$g_{H_2O,ox-atm} = \left(g_{H_2O,ox}^{-1} + g_{H_2O,stomata}^{-1} + g_{H_2O,bl}^{-1} + g_{H_2O,canopy}^{-1} + g_{H_2O,atm}^{-1} \right)^{-1} \quad (6)$$

$g_{H_2O,ox}^{-1}$ includes the resistances of different leaf elements, such as the mesophyll. The computation of $g_{H_2O,stomata}$ and $g_{H_2O,ox}$ are presented in Section 2.1.4. The evaluation of the other H_2O conductances is presented in Appendix C.3.

The area-specific water vapour flow rate ($j_{lat,ox-atm}$ in $\text{cm}^3 \text{cm}^{-2} \text{day}^{-1}$) corresponds to the water flow from the outside of the vascular bundle sheath to the point of measurement of atmospheric variables. It is obtained from Fick's law applied to ideal gases (Tuzet, Perrier, and Leuning 2003; Nobel 2009c):

$$j_{lat,ox-atm} = \frac{Mm_{H_2O}}{\rho_{H_2O}} \times g_{H_2O,ox-atm} \times \left(\frac{ea_{ox} - ea_{atm}}{P_{atm}} \right) \quad (7)$$

With Mm_{H_2O} (kg mmol^{-1}) and ρ_{H_2O} (kg cm^{-3}), respectively, the water molar mass and density, ea (hPa) the actual vapour pressure, P_{atm} (hPa) the atmospheric air pressure. ea_{ox} can be

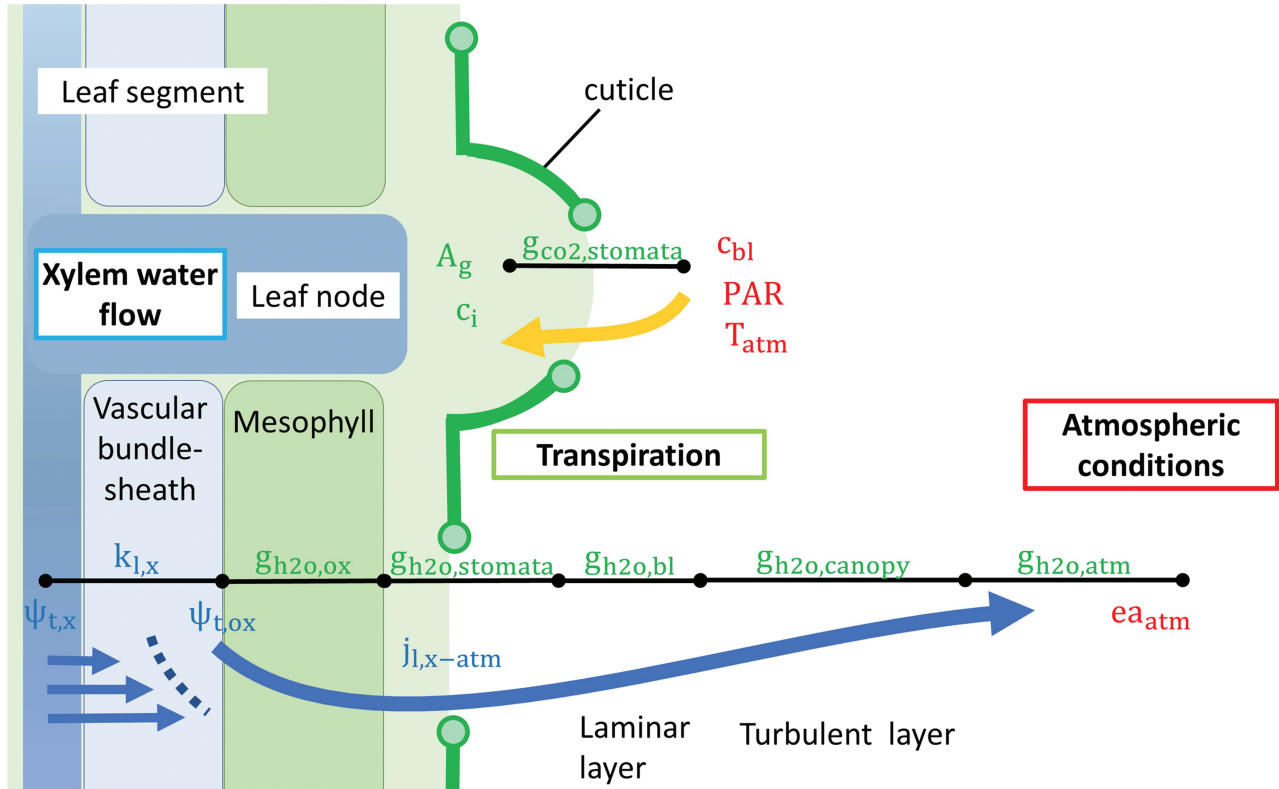


Figure 6. Water flow between the leaf xylem and the point of humidity measurement. The numbering of the image sections was kept identical to those presented in Fig. 1A. The xylem total water potential ($\psi_{t,x}$) varies along the plant segments while each segment has one mean outer-xylem water potential ($\psi_{t,ox}$).

obtained from $\psi_{t,ox}$ using Equation (C6). We do not represent the variations in water storage along the evaporation pathway. We have consequently: $j_{lat,ox-atm} = j_{lat,x-ox} = j_{lat,x-atm}$. All the elements of the considered leaf tissue are at the same height ($\psi_{g,ox} = \psi_{g,x}$) and we neglect the xylem osmotic potential ($\psi_{o,x}$). $\psi_{p,ox}$ can therefore be obtained from

$$\psi_{p,ox} = \psi_{p,x} - \frac{j_{lat,x-atm}}{k_{lat,x}} \quad (8)$$

with $k_{lat,x}$ the lateral conductivity of the vascular bundle sheath ($\text{cm hPa}^{-1} \text{ day}^{-1}$). The exact method used to compute $\psi_{p,ox}$ is presented in Equation (F33).

Carbon assimilation In this section, we present the evaluation of A_n as limited by the rate of carboxylation by Rubisco (F_c in $\text{mmol C cm}^{-2} \text{ day}^{-1}$) and by the rate of RuBP regeneration via electron transport (F_j in $\text{mmol C cm}^{-2} \text{ day}^{-1}$).

Rubisco activity at the sites of carboxylation F_{cmax}^{25} ($\text{mmol cm}^{-2} \text{ day}^{-1}$) corresponds to the maximum F_c for $T = 298.15 \text{ K}$. Qian et al. (2021) defined F_{cmax}^{25} according to the leaf chlorophyll content (Chl in mmol cm^{-2}):

$$F_{cmax}^{25} = k_{chl1} \times Chl + k_{chl2} \quad (9)$$

with k_{chl1} and k_{chl2} fitting parameters representing the empirical relationship between F_{cmax}^{25} and Chl . k_{chl1} and k_{chl2} can be set

according to the assimilation rate when F_c is limiting for photosynthesis. Chl is currently an input parameter and can be used to represent the effect of plant nitrogen uptake.

F_{cmax} ($\text{mmol cm}^{-2} \text{ day}^{-1}$) is the maximal F_c ($\text{mmol cm}^{-2} \text{ day}^{-1}$) at a temperature T :

$$F_{cmax} = F_{cmax}^{25} \times Arrhenius(T_{seg}, E_{a,v}) \times TempInhib(T_{seg}, E_{d,v}) \quad (10)$$

$E_{a,v}$ and $E_{d,v}$ (mJ mmol^{-1}) are, respectively, the activation and deactivation energy for F_{cmax} . $Arrhenius(T_{seg}, E_{a,v})$ represents the result of the Arrhenius function (see Equation (C7)) and $TempInhib(T_{seg}, E_{d,v})$ represents the result of the temperature inhibition function (see Equation (C8)).

F_c is affected by Γ^* ($\text{mmol CO}_2 \text{ mmol air}^{-1}$), the CO_2 compensation point (equilibrium CO_2 level reached when $A_n=0$) in the absence of mitochondrial respiration (R_d in $\text{mmol cm}^{-2} \text{ d}^{-1}$). Γ^* and R_d are obtained from Equation (C9).

F_c follows a Michaelis–Menten function and depends on the CO_2 and O_2 molar fractions in the substomatal cavity, respectively, c_i ($\text{mmol CO}_2 \text{ mmol air}^{-1}$) and o_i ($\text{mmol O}_2 \text{ mmol air}^{-1}$).

F_c can then be computed using Equation (11):

$$F_c = \max \left(F_{cmax} \times \frac{c_i - \Gamma^*}{c_i + M_{CO_2} \left(1 + \frac{o_i}{M_{O_2}} \right)}, 0 \right) \quad (11)$$

With M_{CO_2} and M_{O_2} (mmol mmol⁻¹) the Michaelis coefficients for, respectively, CO₂ and O₂ (see Equation (C9)). The computation of c_i is presented in Section 2.1.4.

Electron transport rate $J_{e_{max}}^{25}$ (mmol cm⁻² day⁻¹) is the maximum electron transport rate for $T = 298.15$ K. It is assumed to be proportional to $F_{c_{max}}^{25}$ (Tuzet, Perrier, and Leuning 2003):

$$J_{e_{max}}^{25} = k_{j_{max}} F_{c_{max}}^{25} \quad (12)$$

with $k_{j_{max}} (-)$ a set coefficient which can be defined according to the light saturation point for photosynthesis under well-watered conditions. $J_{e_{max}}$ (mmol cm⁻² day⁻¹) is the maximum electron transport rate and is computed with the following equation:

$$J_{e_{max}} = J_{e_{max}}^{25} \times Arrhenius(T_{seg}, E_{a,j}) \times TempInhib(T_{seg}, E_{d,j}) \quad (13)$$

with $E_{a,j}$ and $E_{d,j}$ (mJ mmol⁻¹), respectively, the activation and deactivation energy for $J_{e_{max}}$.

We can then obtain Je (mmol cm⁻² day⁻¹), the electron transport rate for a value of photosynthetically active radiation absorbed (PAR in mmol photons cm⁻² day⁻¹):

$$\omega Je^2 - (\alpha PAR + J_{e_{max}}) Je + \alpha PAR \times J_{e_{max}} = 0 \quad (14)$$

with $\omega (-)$ a parameter that determines the shape of the parabola and $\alpha (-)$ the quantum yield of whole-chain electron transport.

Je corresponds to the smaller root of the quadratic equation (Bonan 2019):

$$Je = \frac{\alpha PAR + J_{e_{max}} - \sqrt{(\alpha PAR + J_{e_{max}})^2 - 4\omega \alpha PAR J_{e_{max}}}}{2\omega} \quad (15)$$

From Je , we can compute F_j :

$$F_j = \max\left(\frac{Je}{4} \times \frac{c_i - \Gamma^*}{c_i + 2\Gamma^*}, 0\right) \quad (16)$$

Gross and net assimilation rates The gross and net CO₂ assimilation rates (respectively, A_g and A_n in mmol cm⁻² day⁻¹) correspond to the quantity of sucrose gained by the plant per unit of leaf exchange surface and time. They are computed from F_c (Equation (11)), F_j (Equation (16)) and R_d (Equation (C9)):

$$A_g = \min(F_c, F_j) \quad (17)$$

$$A_n = A_g - R_d \quad (18)$$

A_n is then used as source term for the sucrose flow (see Section 2.1.4). When $A_g < R_d$, we have a negative sucrose source in the mesophyll (see Equation (41)). In such cases, R_d is also limited by the amount of sucrose available in the mesophyll and can be lower than the value obtained from Equation (C9).

Leaf water and CO₂ conductance The molar conductances of the domain Y to CO₂ and H₂O (respectively $g_{CO_2,Y}$ and $g_{H_2O,Y}$ in mmol cm⁻² day⁻¹) correspond to the flow of gaseous CO₂ (resp. H₂O) per unit of CO₂ concentration (resp. water vapour pressure). $g_{CO_2,stomata}$ depends on the gradient between c_i and the CO₂ compensation point (Γ in mmol CO₂ mmol air⁻¹). Γ is obtained from Equation (19).

$$\Gamma = \frac{\Gamma^* + M_{CO_2} R_d \left(1 + \frac{a_i}{M_{O_2}}\right) / F_{c_{max}}}{1 - R_d / F_{c_{max}}} \quad (19)$$

A low $\psi_{t,ox}$ will lead to lower $g_{CO_2,stomata}$ and $g_{H_2O,ox}$. This response is represented empirically via a dimensionless water scarcity factor (f_{w1}):

$$f_{w1} = f_{w1r} + (1 - f_{w1r}) \frac{1 + e^{k_{fw1} \psi_{t,crit,1}}}{1 + e^{k_{fw1} (\psi_{t,crit,1} - \psi_{t,ox})}} \quad (20)$$

with $\psi_{t,crit,1}$ (hPa) the critical water potential. $k_{fw1} (-)$ is a sensitivity parameter. A higher value of k_{fw1} leads to a stronger variation of f_{w1} around $\psi_{t,crit,1}$, whereas a lower value leads to a more gradual response.

$g_{H_2O,ox}$ (mmol cm⁻² day⁻¹), the conductivity to water of the pathway between the xylem membrane and the substomatal cavity, is computed from its maximum value ($g_{H_2O,ox,max}$ assumed constant) and the water scarcity factor f_{w1} : $g_{H_2O,ox} = g_{H_2O,ox,max} \times f_{w1}$.

$g_{H_2O,stomata}$ and $g_{CO_2,stomata}$ are computed following the model of Tuzet, Perrier, and Leuning (2003):

$$g_{H_2O,stomata} = k_{g2,stomata} \times g_{CO_2,stomata} \quad (21)$$

$$g_{CO_2,stomata} = g_{0,CO_2,stomata} + \frac{k_{g1} A_n}{c_i - \Gamma} \times f_{w1} \quad (22)$$

with $g_{0,CO_2,stomata}$ (mmol cm⁻² day⁻¹) the residual stomatal opening. k_{g2} accounts for the H₂O to CO₂ ratio of molecular diffusivity— $k_{g2,stomata} = 1.6$ (Tuzet, Perrier, and Leuning 2003). As opposed to the model of Leuning (1995), the model of Tuzet, Perrier, and Leuning (2003) model uses c_i and not c_{bl} (mmol CO₂ mmol air⁻¹), the CO₂ molar fraction at the leaf surface. Indeed, c_i was shown to have a stronger influence on $g_{CO_2,stomata}$ (Damour et al. 2010). $k_{g1} (-)$ is a fitting parameter representing the effect of A_g on $g_{CO_2,stomata}$. It can be computed from the expected $\frac{c_i}{c_{bl}}$ ratio when $f_{w1} = 1$ using Equation (26) presented in the next section.

Substomatal CO₂ molar fraction Following an Ohm's law adaptation of Fick's law of diffusion, c_i (mmol mmol⁻¹) can be calculated with the 'CO₂ supply function' (Damour et al. 2010; Dewar 2002):

$$c_i = c_{atm} - \frac{A_n}{g_{CO_2,stomata-atm}} \quad (23)$$

with c_{atm} (mmol mmol⁻¹) the CO₂ molar fraction at the point of measurement. However, when A_g is low, our fixed-point iteration solving scheme (see Section 2.1.6) does not converge and gives unrealistic c_i value ($c_i \leq 0$ or $c_i \gg c_{bl}$). For this reason,

similarly to Dewar (2002), we use the CO₂ molar fraction on the leaf surface (c_{bl} in mmol mmol^{-1}).

$$c_i = c_{bl} - \frac{A_n}{g_{\text{CO}_2, \text{stomata}}} \quad (24)$$

With c_{bl} an input parameter.

We then combine Equations (22) and (24) and we neglect $g_{0, \text{CO}_2, \text{stomata}}$:

$$c_i - c_{bl} = \frac{A_n}{\frac{k_{g1} A_n}{c_i - \Gamma} \times f_{w1}} \quad (25)$$

$$c_i = \frac{c_{bl} k_{g1} f_{w1} + \Gamma}{1 + k_{g1} f_{w1}} \quad (26)$$

If we assume that c_{bl} and k_{g1} are set parameters and $\Gamma \ll c_{bl}$, the c_i value then mainly depends on f_{w1} (–), the water scarcity factor of the stomatal model. This follows field observations, where $\frac{c_{bl}}{c_i}$ is usually seen to be constant, except in case of water scarcity (Damour et al. 2010).

Xylem water flow Darcy's law is seen as a good approximation to compute the axial flux of water in the xylem ($J_{ax,x}$ in $\text{cm}^3 \text{d}^{-1}$) (Roose and Fowler 2004). Moreover, we assume that the xylem solution has physical characteristics similar to that of pure water. We, therefore, neglect $\psi_{o,x}$ (hPa), the xylem osmotic potential. We thus have $\psi_{t,x} = \psi_{p,x} + \psi_{g,x}$, with $\psi_{t,x}$ the total xylem solution potential, $\psi_{p,x}$ the xylem hydrostatic potential and $\psi_{g,x}$ the gravitational potential, all in hPa. For a straight xylem segment, we obtain:

$$J_{ax,x} = -K_{ax,x} \left(\frac{\partial \psi_{p,x}}{\partial \xi} + \frac{\partial \psi_{g,x}}{\partial \xi} \right), \quad (27)$$

$$J_{ax,x} = -K_{ax,x} \frac{\partial \psi_{t,x}}{\partial \xi}, \quad (28)$$

$$K_{ax,x} = \frac{\pi}{8\mu_{\text{H}_2\text{O}}} \times \sum_i^{n_x} a_{x,i}^4 \quad (29)$$

$K_{ax,x}$ ($\text{cm}^4 \text{hPa}^{-1} \text{day}^{-1}$) is the xylem intrinsic axial conductance and ξ (cm) corresponds to the local axial coordinate of the plant. $\mu_{\text{H}_2\text{O}}$ (hPa day) is the temperature-dependent viscosity of pure water. $a_{x,i}$ (cm) is the radius of the xylem vessel number i in the segment cross-section and n_x is the number of xylem vessels in the cross-section.

The sink and source for water are given by the lateral water flow ($j_{\text{lat},x\text{-out}}$ in cm day^{-1}), which corresponds to the xylem–soil ($j_{\text{lat},x\text{-soil}}$) or xylem–atmosphere ($j_{\text{lat},x\text{-atm}}$) water exchange:

$$j_{\text{lat},x\text{-out}} = \begin{cases} j_{\text{lat},x\text{-soil}} = k_{\text{lat},x}(\psi_{p,x} - \psi_{m,\text{soil}}), & \text{if root} \\ j_{\text{lat},x\text{-atm}} = k_{\text{lat},x}(\psi_{p,x} - \psi_{p,\text{ox}}), & \text{if leaf blade,} \end{cases} \quad (30)$$

where $k_{\text{lat},x}$ ($\text{cm hPa}^{-1} \text{day}^{-1}$) is the lateral hydraulic conductivity of the root cortex (for roots) or of the vascular bundle sheath (for leaves). $\psi_{m,\text{soil}}$ is the soil matrix water potential in hPa. $\psi_{m,\text{soil}}$ is given by the soil water flow module (see Section 2.1.5) and $\psi_{p,\text{ox}}$ is given by the FvCB–stomatal regulation module (see

Section 2.1.4, Equation 8). CPlantBox offers several options for setting $k_{\text{lat},x}$ and $K_{ax,x}$ (constant, age dependent, organ type dependent, etc.). $j_{\text{lat},x\text{-out}} > 0$ represents a water loss for the plant.

We do not currently represent the effect of cavitation on the xylem conductivity. Likewise, we do not represent the effect of the water flow between the phloem and the xylem on the xylem water balance. This lateral water exchange is very low when compared with the xylem flow during the day (Zhou et al. 2020; Windt et al. 2006; Hölttä et al. 2006, Fig. 2B). However, because of this simplification, we cannot simulate the ‘Münch's counterflow’ (xylem water flux driven by the phloem water flux) although it is the main force driving the xylem solution at night (Zhou et al. 2020; Windt et al. 2006; Hölttä et al. 2006, Fig. 2B). However, this flow remains low and has a limited effect on our output variables of interest (transpiration rate, growth rate and carbon partitioning).

We neglect the variation of water storage in the plant. The mass balance gives the following driving equation for the xylem solution flow (see Fig. 1A.6):

$$-K_{ax,x} \frac{\partial^2 \psi_{p,x}}{\partial \xi^2} = -p_{\text{seg}} \times j_{\text{lat},x\text{-out}} \text{ for } \Omega \setminus \partial\Omega, \quad (31)$$

$$\frac{\partial \psi_{p,x}}{\partial \xi} = 0 \text{ for } \partial\Omega \text{ (all organ end-nodes)} \quad (32)$$

with p_{seg} (cm) the perimeter of the plant exchange zone, Ω the domain considered (here the plant), and $\partial\Omega$, the domain's boundary (here the tip or end node of each organ). Thus, the soil (Section 2.1.5, Fig. 1A.3), xylem (Fig. 1A.6), and photosynthesis–stomatal opening subproblems (Section 2.1.4, Fig. 1A.4b) are coupled via Equation (31).

Sucrose balance In the following section, we present the equations defining the plant sucrose dynamic (Fig. 1A.5), yielding the sucrose concentration in the sieve tube (s_{st} in $\text{mmol sucrose cm}^{-3}$) and in the leaf mesophyll (s_{meso} in $\text{mmol sucrose cm}^{-3}$). The flow and concentration of sucrose in other tissues (such as the parenchyma) are not explicitly represented. The module also yields $[F_{\text{out}}]$ ($\text{mmol sucrose cm}^{-3} \text{day}^{-1}$), the s_{st} loss rate, which gives the exudation rate and the plant water- and carbon-limited growth (see Section 2.1.4).

Sucrose in the phloem Similarly, to Section 2.1.4, we compute $J_{ax,st}$ ($\text{cm}^3 \text{day}^{-1}$), the sieve tube axial solution flow, by implementing Darcy's law (see Equation (27)). We therefore obtain (M. Thompson and N. Holbrook 2003):

$$J_{ax,st} = -K_{ax,st} \left(\frac{\partial \psi_{p,st}}{\partial \xi} + \frac{\partial \psi_{g,st}}{\partial \xi} \right) \quad (33)$$

$$K_{ax,st} = \frac{\pi}{8\mu_{\text{st}}} \times \sum_i^{n_{\text{st}}} a_{\text{st},i}^4 \times \beta \quad (34)$$

$K_{ax,st}$ ($\text{cm}^4 \text{hPa}^{-1} \text{day}^{-1}$) is the sieve tube axial intrinsic conductance and $\psi_{p,st}$ (hPa) is the sieve tube hydrostatic pressure.

μ_{st} (hPa day) is the viscosity of the sieve tube solution and it is computed from the temperature and sucrose concentration according to the method of Mathlouthi and Génotelle (1995,

Equation (6.29)) as implemented by [Lacointe and Peter E. H. Minchin \(2019\)](#). $a_{st,i}$ (cm) is the radius of the sieve tube number i in the segment cross section and n_{st} is the number of sieve tubes in the cross section.

Following the recommendation of [M. Thompson and N. Holbrook \(2003\)](#), we added the parameter β (–) to the computation of $K_{ax,st}$ to represent the ratio of axial conductance with sieve plates to that without. β can be evaluated via empirical data or from images of phloem and sieve plates ([M. Thompson and N. Holbrook 2003](#)). This parameter is not needed for the xylem tissues as the opening in its cells' end walls are much larger ([Nobel 2009a](#)). CPlantBox offers several options for defining a_{st} (constant, organ type dependent, etc.).

We assumed water equilibrium between the xylem and phloem [[Appendix D](#) for more explanations]. We therefore obtain:

$$\psi_{t,st} = \psi_{t,x} \quad (35)$$

We assume that there is a semi-permeable membrane (permeable to water but not to sucrose) between the phloem and the xylem. The total potential in the phloem, $\psi_{t,st}$, is equal to the sum of sieve tube solution's hydrostatic ($\psi_{p,st}$ hPa), gravitational ($\psi_{g,st}$ hPa) and osmotic potential ($\psi_{o,st}$ hPa). We consequently obtain:

$$\psi_{p,st} + \psi_{g,st} = \psi_{t,x} - \psi_{o,st} \quad (36)$$

We consider that sucrose makes up the largest fraction of solutes in the sieve tube solution ([De Schepper et al. 2013](#)). The $\psi_{o,st}$ can, therefore, be computed according to van't Hoff relation: $\psi_{o,st} = -RT_{seg} s_{st}$. With T_{seg} the segment's temperature in K. As explained by [Hall and P. E. H. Minchin \(2013\)](#) and [Cabrita \(2011, Section 2.2.3.1\)](#), the van't Hoff relation may not be appropriate when $s_{st} > 0.5$ mmol sucrose cm^{-3} . We kept nonetheless that definition of $\psi_{o,st}$ for this first implementation of the model.

Equation (33) becomes:

$$J_{ax,st} = -K_{ax,st} \left(\frac{\partial \psi_{t,x}}{\partial \xi} + RT_{seg} \frac{\partial s_{st}}{\partial \xi} \right) \quad (37)$$

Using the relations defined above, we do not need to solve another equation for $\psi_{p,st}$, but can at all times compute it from other known state variables, namely $\psi_{t,x}$ (see [Equation \(31\)](#)) and s_{st} .

Assuming then that sucrose is transported within the phloem by advection only, with no lateral gradient, constant initial conditions and no-flux boundary conditions, we obtain:

$$\frac{\partial s_{st}}{\partial t} + \frac{\partial}{\partial \xi} \left(s_{st} \times K_{ax,st} \left(RT_{seg} \frac{\partial s_{st}}{\partial \xi} + \frac{\partial \psi_{t,x}}{\partial \xi} \right) - [F_{in}] + [F_{out}] + \frac{\partial starch_{st}}{\partial t} \right) = 0 \text{ for } \Omega \setminus \partial \Omega, \quad t > t_0, \quad (38)$$

$$s_{st} = s_{st,0} \text{ for } t = t_0, \quad (39)$$

$$K_{ax,st} \left(RT_{seg} \frac{\partial s_{st}}{\partial \xi} + \frac{\partial \psi_{t,x}}{\partial \xi} \right) = 0 \text{ for } \partial \Omega \quad (40)$$

with $[F_{in}]$ and $[F_{out}]$ (mmol sucrose $\text{cm}^{-3} \text{d}^{-1}$), respectively, the source and sink of s_{st} (see [Sections 2.1.4](#) and [2.1.4](#), respectively),

$starch_{st}$ (mmol sucrose cm^{-3}) the concentration of starch in the sieve tube (see [Sections 2.1.4](#)), and t_0 the time at the beginning of the simulation.

Sucrose in the mesophyll Like s_{st} , we solve s_{meso} (mmol sucrose cm^{-3}), the sucrose concentration in the leaf source compartments (considered to be the mesophyll cells). As represented in [Fig. 1A.5a](#), A_n is obtained from the photosynthesis module (see [Section 2.1.4](#)) and leads to a variation of s_{meso} . Then occurs an active phloem loading from the mesophyll to the sieve tube ($[F_{in}]$ in mmol sucrose $\text{cm}^{-3} \text{d}^{-1}$) ([De Schepper et al. 2013](#)), defined according to [Stanfield and Bartlett \(2022\)](#). We do not simulate axial flow within the mesophyll compartments. In summary:

$$\frac{\partial s_{meso}}{\partial t} = \frac{A_n p_{blade} \times l}{12 v_{meso}} - [F_{in}] - \frac{\partial starch_{meso}}{\partial t}, \text{ for } t > t_0 \quad (41)$$

$$s_{meso} = s_{meso,0} \text{ for } t = t_0, \quad (42)$$

$$[F_{in}] = \frac{F_{in,max}}{v_{st}} \times \frac{s_{meso}}{M_{meso} + s_{meso}} \times e^{-\beta_{meso} s_{st}} \quad (43)$$

p_{blade} (cm) and v_{meso} (cm^3) are, respectively, the leaf blade perimeter and mesophyll volume. The factor 12 allows us to go from mmol C d^{-1} to mmol sucrose d^{-1} . $F_{in,max}$ (mmol sucrose day^{-1}) is the maximum loading rate into the sieve tube, β_{meso} (–) is a factor indicating the strength of the s_{st} down-regulation for loading. M_{meso} (mmol sucrose cm^{-3}) is the Michaelis–Menten coefficient for the sucrose loading. $starch_{meso}$ (mmol sucrose cm^{-3}) is the concentration of starch in the mesophyll (see [Sections 2.1.4](#)). When $A_n < 0$, the sucrose in the mesophyll is used for mitochondrial respiration (R_d , see [Equation \(C9\)](#)).

Sucrose storage We represent the storage of sucrose as starch ($s_{starch,X}$ in mmol sucrose cm^{-3}) via [Equation \(44\)](#), taken from [Lacointe and Peter E. H. Minchin \(2019\)](#):

$$\frac{\partial starch_X}{\partial t} = \frac{F_{max,starch,X} \times s_X}{M_{starch,X} + s_X} - k_{hyd,starch,X} \times starch_X + k_{targ,starch,X} (s_X - s_{targ,X}) \quad (44)$$

with the X subscript standing for st or $meso$. As [Lacointe and Peter E. H. Minchin \(2019\)](#) explained in their paper, this equation allows the user to represent several dynamic. A Michaelis–Menten synthesis dynamic can be represented by setting a non-zero (i) maximum value of starch synthesis ($F_{max,starch,X}$ in mmol sucrose $\text{cm}^{-3} \text{d}^{-1}$) and (ii) Michaelis constant ($M_{starch,X}$ in mmol sucrose cm^{-3}). Relative starch hydrolyse rate is given by $k_{hyd,starch,X}$ (d^{-1}). Starch metabolism is dependent on a target s_X ($s_{targ,X}$ in mmol sucrose cm^{-3}) if the related constant $k_{targ,starch,X}$ (d^{-1}) is not null.

Sucrose usage In this section, we present how to compute the maximal or water-limited sucrose usage rates for each sink category. From this, we obtain the total sucrose sink term ($[F_{out}]$ in mmol sucrose $\text{cm}^{-3} \text{d}^{-1}$) used in the s_{st} balance equation (see

Equation (38) and Fig. 1A.7). We also present how $[F_{\text{out}}]$ is used to compute the realized (s_{st} -limited) sinks (Fig. 1A.2b).

In the plants, s_{st} can be used for growth (Gr , in mmol sucrose day^{-1}), root exudation ($Exud$, in mmol sucrose day^{-1}) and respiration (Dilkes, D. L. Jones, and Farrar 2004; J. H. M. Thornley and Cannell 2000; Galindo-Castañeda et al. 2022). s_{st} respiration can be divided in two conceptual categories: growth respiration (R_{gr} , in mmol sucrose day^{-1}), which is linked to Gr , and maintenance (or residual) respiration (R_m , in mmol sucrose day^{-1}). This conceptual representation follows the growth-maintenance paradigm (Roux et al. 2001; J. H. M. Thornley and Cannell 2000; Amthor 2000). Other sucrose sinks, notably starch synthesis, are not represented (discussed in Section 4.3). Each carbon sink X (mmol sucrose day^{-1}) can also be given in concentration units (with $[X]$ in mmol sucrose cm^{-3} day^{-1}), obtained from $[X] = \frac{X}{v_{\text{st}}}$, with v_{st} (cm^3) the volume of the sieve tube.

Exudation The root exudation rate ($Exud$, in mmol sucrose day^{-1}) is assumed to be a passive process (Galindo-Castañeda et al. 2022), dependent on the lateral sucrose gradient:

$$Exud = k_{\text{lat,st}} \times p_{\text{seg}} \times l \times \max(\bar{s}_{\text{st}} - s_{\text{soil}}, 0) \quad (45)$$

$$\bar{s}_{\text{st}} = \min(s_{\text{st}} - s_{\text{st,min}}, 0) \quad (46)$$

with $k_{\text{lat,st}}$ (cm d^{-1}) the lateral sieve tube conductivity for sucrose. Similarly to $k_{\text{lat,x}}$, CPlantBox offers several options for setting $k_{\text{lat,st}}$ (constant, root order dependent, etc.). s_{soil} (mmol sucrose cm^{-3}) is the mean soil carbon concentration in equivalent sucrose. l (in cm) is the evaluated length. $s_{\text{st,min}}$ (mmol sucrose cm^{-3}) is the minimum sucrose concentration below which no usage of sucrose occurs. This parameter allows the user to define more easily a minimum sucrose concentration to follow experimental observations and to respect the necessary conditions for water equilibrium between xylem and phloem (Appendix D).

Water-limited growth and growth respiration The water-limited (or potential) growth-related sink ($G_{\text{tot,Wlim}}$, in mmol sucrose day^{-1}) corresponds to the potential carbon used for growth (Gr_{Wlim}) and growth-related respiration ($R_{gr,Wlim}$). It is computed as follows:

$$G_{\text{tot,Wlim}} = R_{gr,Wlim} + Gr_{\text{Wlim}}, \quad (47)$$

$$Gr_{\text{Wlim}} = r_{\text{Wlim}} \rho_s A_{\text{cross,seg}}, \quad (48)$$

$$R_{gr,Wlim} = Gr_{\text{Wlim}} \frac{1 - Y}{Y} \quad (49)$$

with Y (—), the sucrose use efficiency for growth. ρ_s (mmol sucrose cm^{-3}) is the volumetric structural carbon content of this tissue in unit of sucrose. $A_{\text{cross,seg}}$ (cm^2) is the cross-sectional area of the segment. r_{Wlim} (cm d^{-1}) is the water-limited growth rate, computed via Equation (2).

Maximal maintenance respiration $R_{m,\text{max}}$ (mmol sucrose cm^{-3} day^{-1}) corresponds to the maximal (non-carbon limited) value of R_m . It represents, for instance, the sucrose usage to replace the

structural carbon (re-synthesis), secondary growth, the phloem leakage and futile cycles (J. H. M. Thornley and Cannell 2000; Lacoite and Peter E. H. Minchin 2019). $R_{m,\text{max}}$ is obtained empirically from Equation (50):

$$R_{m,\text{max}} = v_{\text{seg}} (\rho_s k_{m1} + \bar{s}_{\text{st}} \times k_{m2}) \times Q10^{\frac{T - T_{\text{refq10}}}{10}} \quad (50)$$

with v_{seg} (cm^3) the volume of the plant tissues. k_{m1} , k_{m2} are fitting parameters defining $R_{m,\text{max}}$ according to, respectively, the structural (for wall re-synthesis) and non-structural carbon contents. Following the example of Gauthier et al. (2020), we added the short-term effect of temperature on $R_{m,\text{max}}$ via $Q10$ (—) and T_{refq10} (K) (Amthor 2000). $Q10$ is a coefficient which is widely used in the scientific literature and which defines the temperature sensitivity of chemical reactions: higher $Q10$ value leads to steeper increase with temperature. T_{refq10} defines the reference temperature: $|Q10^{\frac{T - T_{\text{refq10}}}{10}}|_{T=T_{\text{refq10}}} = 1$. As other modules are added to CPlantBox (like nitrogen uptake and flow), their related respiration may be added to the computation of $R_{m,\text{max}}$.

Sucrose-limited sinks $[F_{\text{out,MM}}]$ (mmol sucrose cm^{-3} day^{-1}) is the sucrose usage rate for growth and maintenance. It follows a saturation dynamic and is computed from the Michaelis–Menten response function (Gauthier et al. 2020; S. Jones and Cox 2019; Lacoite and Peter E. H. Minchin 2019):

$$[F_{\text{out,MM}}] = ([R_{m,\text{max}}] + [G_{\text{tot,Wlim}}]) \times \frac{\bar{s}_{\text{st}}}{\bar{s}_{\text{st}} + M_{\text{out}}}, \quad (51)$$

with M_{out} the Michaelis–Menten coefficient. After adding the passive $Exud$, we obtain $[F_{\text{out}}]$ (mmol sucrose cm^{-3} day^{-1}) the total sucrose usage rate:

$$[F_{\text{out}}] = [F_{\text{out,MM}}] + [Exud] \quad (52)$$

A high increase in s_{st} will only affect the maintenance and growth rate if the sink cells are not saturated, while the exudation will not be demand limited.

$F_{\text{out,MM}}$ gives us the value of $[R_m]$ and $[G_{\text{tot,CWlim}}]$ (mmol sucrose cm^{-3} day^{-1}), the realized sucrose usage rate for maintenance and growth respectively:

$$[R_m] = \min([R_{m,\text{max}}], [F_{\text{out,MM}}]) \quad (53)$$

$$[G_{\text{tot,CWlim}}] = [F_{\text{out,MM}}] - [R_m] \quad (54)$$

Equation (53) indicates that maintenance has priority over growth, which is a common assumption (Roux et al. 2001, Fig. 1).

2.1.5. Soil water flow

The variation in soil water content ($\frac{\partial \theta_{\text{soil}}}{\partial t}$) is computed, thanks to the DuMu^x module (see Fig. 1A.3) using the Richards equation,

which describes the movement of water in an unsaturated soil (Richards 1931; Koch et al. 2021):

$$\frac{\partial \theta_{\text{soil}}}{\partial t} - \nabla \cdot (\kappa_{\text{soil}}(\theta_{\text{soil}})(\nabla \psi_{m,\text{soil}} + \nabla \psi_{g,\text{soil}})) = \frac{1}{V_{\text{soil}}} \sum_i^N (p_i \times l_i \times j_{\text{lat},x,\text{soil},i}) \quad (55)$$

with $\sum_i^N (p_i \times l_i \times j_{\text{lat},x,\text{soil},i})$, the root–soil water exchange for all roots i in the considered soil domain (Neumann boundary condition obtained from Section 2.1.4), V_{soil} (cm^3) the volume of the considered soil domain, and $\kappa_{\text{soil}}(\theta_{\text{soil}})$ (in $\text{cm}^2 \text{ hPa}^{-1} \text{ d}^{-1}$) the soil conductivity for a specific water content.

The soil water content (θ_{soil} in $\text{cm}^3 \text{ cm}^{-3}$) and $\kappa_{\text{soil}}(\theta_{\text{soil}})$ are obtained from the van Genuchten–Mualem equations (Mualem 1976; Genuchten 1980):

$$\theta_{\text{soil}} = \theta_{r,\text{soil}} + \frac{\theta_{s,\text{soil}} - \theta_{r,\text{soil}}}{\left[1 + (\alpha_{\text{soil}} |\psi_{m,\text{soil}}|)^{n_{\text{soil}}}\right]^{m_{\text{soil}}}} \text{ if } \psi_{m,\text{soil}} < 0 \quad (56)$$

$$\theta_{\text{soil}} = \theta_{s,\text{soil}} \text{ if } \psi_{m,\text{soil}} \geq 0 \quad (57)$$

$$\kappa_{\text{soil}}(\theta_{\text{soil}}) = \kappa_{\text{soil}}(\theta_{s,\text{soil}}) \frac{\left(1 - (\alpha_{\text{soil}} |\psi_{m,\text{soil}}|)^{n_{\text{soil}}-1} \left[1 + (\alpha_{\text{soil}} |\psi_{m,\text{soil}}|)^{n_{\text{soil}}}\right]^{-m_{\text{soil}}}\right)^2}{\left[1 + (\alpha_{\text{soil}} |\psi_{m,\text{soil}}|)^{n_{\text{soil}}}\right]^{m_{\text{soil}}/2}} \quad (58)$$

$$\psi_{m,\text{soil}} = \psi_{m,\text{soil},0} \text{ for } t = t_0 \quad (59)$$

$$m_{\text{soil}} = 1 - \frac{1}{n_{\text{soil}}} \quad (60)$$

with α_{soil} (hPa^{-1}) a parameter related to the inverse of the air-entry suction, n_{soil} and m_{soil} (–) parameters representing the soil pore-size distribution, $\theta_{s,\text{soil}}$ and $\theta_{r,\text{soil}}$ ($\text{cm}^3 \text{ cm}^{-3}$) the saturated and residual soil water contents, $\kappa_{\text{soil}}(\theta_{s,\text{soil}})$ (in $\text{cm}^2 \text{ hPa}^{-1} \text{ day}^{-1}$) the saturated soil conductivity. We neglect the effect of $\psi_{o,\text{soil}}$ and $\psi_{o,x}$ (the osmotic potential in the soil and in the xylem) on the flow. $\psi_{m,\text{soil}}$ can thus be used by the xylem module (Dirichlet boundary condition), see Equation (30). The coupling between CPlantBox and DuMu^x is made available via a python binding within the root–soil interaction module DuMu^x-ROSI (Khare et al. 2022). The method for the soil discretization and interface with the xylem flow is given in Appendix F.2.1.

We do not represent in this implementation the variation of soil carbon concentration.

2.1.6. Numerical solution and computational loop

The numerical solutions of each CPlantBox modules and of the DuMu^x soil water flow module are described in Appendix F and in Koch et al. (2021), respectively. Briefly, the soil water flow is solved by a cell-centred finite volume method (CC-FVM) (Koch et al. 2021). The xylem water flow is solved using the hybrid analytical method of Meunier et al. (2017). The sucrose balance (sucrose usage and transport in the sieve tube and mesophyll) is computed by discretizing the continuous equation into

a series of ODEs solved numerically (Newton iterations with implicit time stepping) on each plant node (vertex-centred finite volume method, VC-FVM) (Hindmarsh et al. 2005). The xylem water flow and FvCB-stomatal regulation are computed together via fixed-point iterations. For these two modules, an iterative calculation of c_i , A_g , g_{CO_2} , $j_{\text{lat},x-\text{out}}$, $\psi_{t,ox}$ and $\psi_{t,x}$ for each plant segment is carried out (in that order). Convergence is said to have been reached when the relative difference between two consecutive loops in each segment for each of these variables is below 1% or when the absolute difference is below a set threshold. The other modules are run sequentially at each user-defined time step. The user can run all the modules at each loop or increase the time step of some modules by running them every set number of loops (operator splitting). The optimal time step for the data exchange between the modules is strongly problem dependent and to be selected by trial and error. Figure 7 gives a graphical representation of the simulation loop and main exchange of data between the modules.

2.2. System modelled

The model was calibrated for C3 monocots using experimental Appendix E.1], literature or illustrative data. The list of the parameters, with their value and source, is given in Appendix E.2.

Notably, for this implementation, different $k_{\text{lat},\text{st},\text{root}}$ and $k_{\text{lat},x,\text{root}}$ were defined for each root order. Moreover, we set

$$k_{\text{lat},\text{root},l} > 0 \text{ if } l \in [0, l_{\text{rootExchange}}]$$

where l is the distance from the root tip and $l_{\text{rootExchange}} = 0.8 \text{ cm}$. This means that root water uptake and exudation are assumed to occur in the immature portion of the root (Bramley 2006, Chap. 4).

We simulated the growth of a C3 monocot under a control scenario (hereafter called *baseline*) compared with dry spells at two stages of the development of the plant.

The environmental variables (see Table 1) of *baseline* (resp. the dry spell periods) were set from the data of Swart et al. (2019) for Germany in June of 2010 (resp. 2100, under the SSP5–8.5 scenario), making *baseline* relatively wetter and colder (resp. the dry spell periods relatively drier and warmer). $\theta_{\text{mean},\text{soil}}$ for *baseline* was set near saturation. $\theta_{\text{mean},\text{soil}}$ during the dry spells was set 30% lower, which corresponds to the relative decrease in moisture in the upper soil column between June 2010 and 2100 (Swart et al. 2019).

Both dry spells were represented by a period of 1 week without rainfall: 11–18 days and 18–25 days after sowing, hereafter called *early dry spell* and *late dry spell*.

The virtual plants were obtained by running CPlantBox 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. Indeed, the plant leaf blades (the carbon source and water sink) had to be large enough before starting the carbon- and water-limited growth. After 3 h of burn-in time, we simulated the carbon and water fluxes and of the carbon- and water-limited growth. The plants all grew under the *baseline* conditions with a static soil (constant mean $\psi_{m,\text{soil}} = 0.4 \text{ cm}^3 \text{ cm}^{-3}$ at hydraulic equilibrium), except during the dry spell between Day 10 and (for *early dry spell*, resp. *late dry*

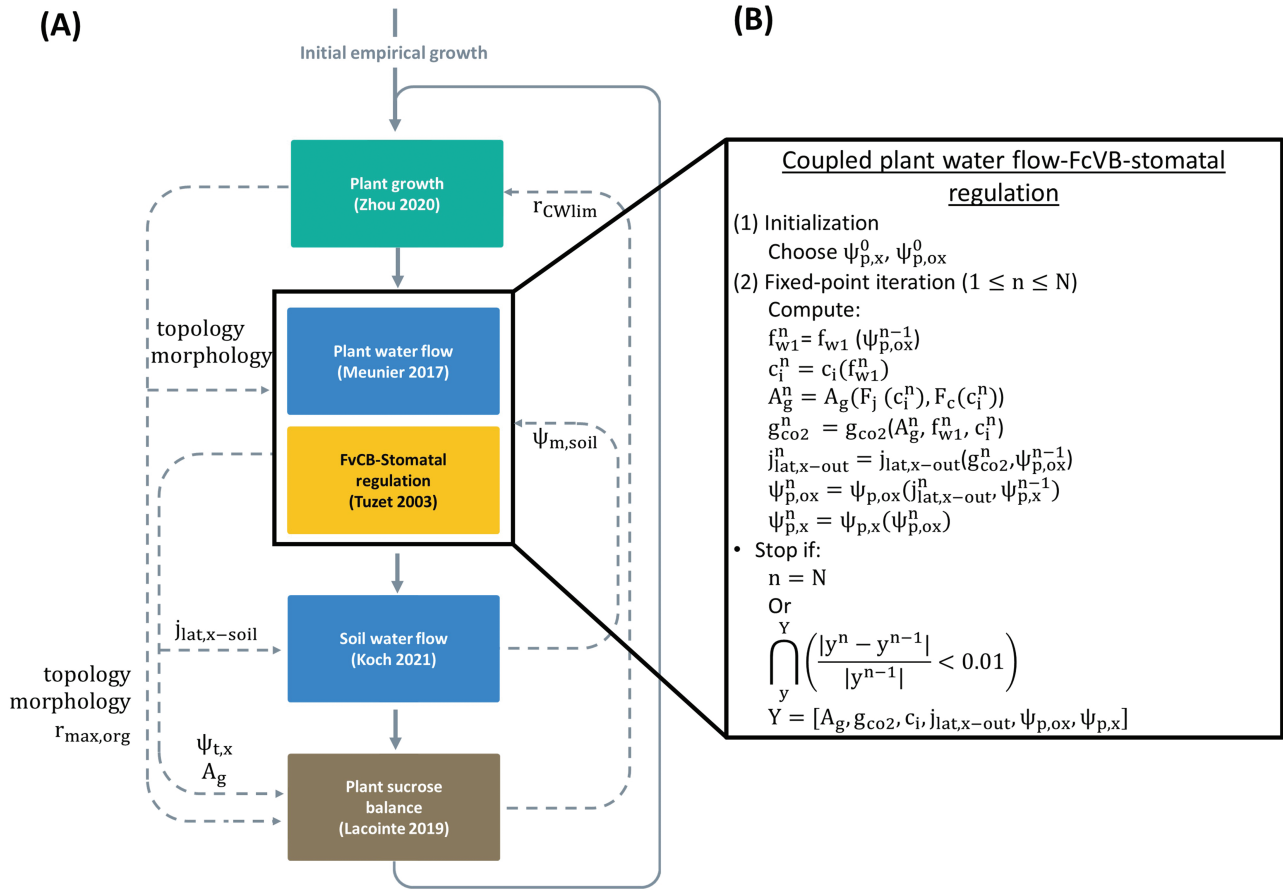


Figure 7. Representation of the simulation loop of the model with (A) the overall loop, and (B) the fixed-point iteration loop used for the coupled plant water flow–FvCB–stomatal regulation modules. The dashed arrows represent the exchange of data between the modules. The full arrows give the sequence of the modules in the loop. At each time step, each part of the model is computed sequentially, except for the water flow–FvCB–stomatal regulation modules which are looped over until convergence.

Table 1. Environmental variables

	Min–max of sinusoidal function ^a			$\theta_{mean,soil}$
	PAR	T_{atm} (K)	h_{atm}^b (%)	($cm^3 cm^{-3}$)
baseline	0–940	288.95–295.15	0.6–0.88	0.4
dry spell		293.85–303.42	0.44–0.74	0.28

^a T_{atm} , PAR and h_{atm} go from their minimum to their maximum value via a sinusoidal function with a period of 1 day to represent the day–night cycle. All the atmospheric variables correspond to values 2 m aboveground.

^b Relative air humidity.

The *baseline* variables were used for all simulations before and after the dry spells.

spell) the start of the dry spells (11d, resp. 18 days). At the start of the dry spells, the dynamic soil water flow module was implemented. For the plants under *drier&warmer*, the alternative initial soil conditions were used (initial $\psi_{m,soil} = 0.28 cm^3 cm^{-3}$). The soil water flow was simulated until the end of the dry spells (18 days, resp. 25 days). After the dry spells, the *baseline* environmental and static soil variables were used. Table 2 summarizes the above-given timeline of the four simulations.

The minimum plant segment length was set to 1 cm. The θ_{soil} per voxel is (until the start of the dry spells) constant per layer and varies with the depth (hydraulic equilibrium). The mean

Table 2. Timeline of the simulations. The grey (resp. blue) cells between days 1 and 9 (resp. 10 and 25) indicate the empirical (resp. semi-mechanistic) growth period and “ds” the implementation of the dynamic soil. The blue gradient during the dynamic soil simulation represent 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 represent the implementation of the *dry spell* (resp. *baseline*) atmospheric and initial (resp. constant) soil variables.

scenario	day after sowing			
	1...9	10	9...18	18...25
baseline				
early dry spell		ds		
late dry spell				ds

θ_{soil} value is given in Table 1. The voxel size (resolution) was set to $1 cm^3$.

The Van Genuchten parameters are presented in Appendix E.2 and Supporting Information—Table 4. The mean soil-soluble carbon concentration was set as a unique constant value. In order to represent the effect of the water uptake by neighbouring

root systems, we defined the lateral dimensions of the simulation domain to be equal to the inter-plant distance, $3 \times 12 \text{ cm}^2$, and used a laterally periodic domain. The depth of the simulation domain was 60 cm. During the dynamic soil simulation, no rainfall occurred and we assumed that the soil was covered with gravel (negligible evaporation). We could thus set a no-flux upper boundary condition for the soil water-flow module. We, moreover, set a free-flow lower boundary condition.

Although we represented the air humidity gradient between the middle of the canopy and the point of measurement, the atmospheric conditions were represented by a set of mean values, equal for the whole canopy. This means that the same c_{bl} , PAR , T_{atm} and ea_{atm} were set for all shoot segments. We assumed a constant wind speed 2 m above ground u_{2m} of $8.467e + 7 \text{ cm day}^{-1}$ (or 2 m s^{-1} in SI units). The CO_2 concentration on the leaf surface (c_{bl}) was set constant at $350e - 6 \text{ mmol mmol}$, an illustrative value based on measurements from the TERENO- observatory network in Selhausen (Puetz et al. 2016). We simulated a unified temperature in the whole system $T_{plant} = T_{soil} = T_{atm}$. PAR , T_{atm} and h_{atm} (relative air humidity 2 m aboveground) went from their minimum to their maximum value via a sinusoidal function with a period of 1 day.

The time step for the main simulation loop was of 1 h. Within this loop, the time step for the exchange of data between the plant and the soil water modules was 1 min.

3. RESULTS

3.1. Simulation of the time course of water and carbon flows

The model was implemented on a Lenovo Thinkpad T490, with an Intel(R) Core(TM) i5-8265U processor, using the Windows subsystem linux Ubuntu20.04. The run time of the simulation was about 1 h 10 min for *baseline*, 2 h 40 min for *early dry spell* and 5 h 25 min for *late dry spell*. The number of plant nodes went up to 2448 (for *baseline*). The relatively high run time of the simulation was linked to the high number of nodes and will be lower for plants with smaller root systems or when decreasing the resolution (increasing the minimum plant segment length).

Figure 8 illustrates the simulated plant structure and output by the model. Figure 8A shows a 3D visualization of the monocot at 18 days for *baseline*.

Figure 8B shows examples of run-time variables for selected nodes: the total water potential in the xylem ($\psi_{t,x}$ in cm) and the mean concentration of sucrose in the sieve tubes (s_{st} in mmol cm^{-3}).

The development of the plant led to a higher $\psi_{t,x}$ because of the improved water uptake capacity. We can also observe an increased gradient of s_{st} between the shoot and roots.

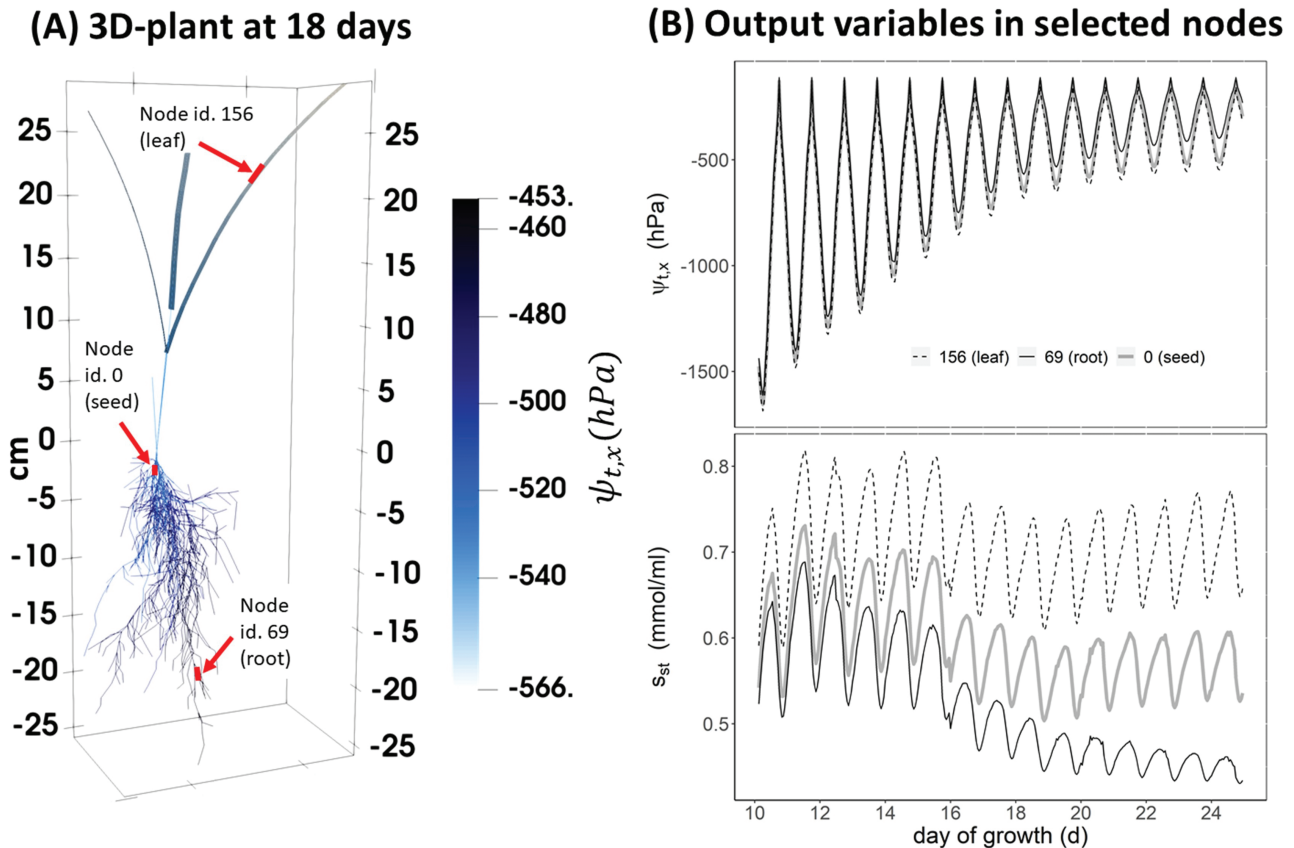


Figure 8. Representation of some CPlantBox outputs at the end of a simulation (A) a 3D image of a C3 monocot at 18 days under *baseline*; (B) values for three specific plant nodes of the xylem water potential ($\psi_{t,x}$) and phloem sucrose concentration (s_{st}). The red arrows and rectangles indicate the selected nodes.

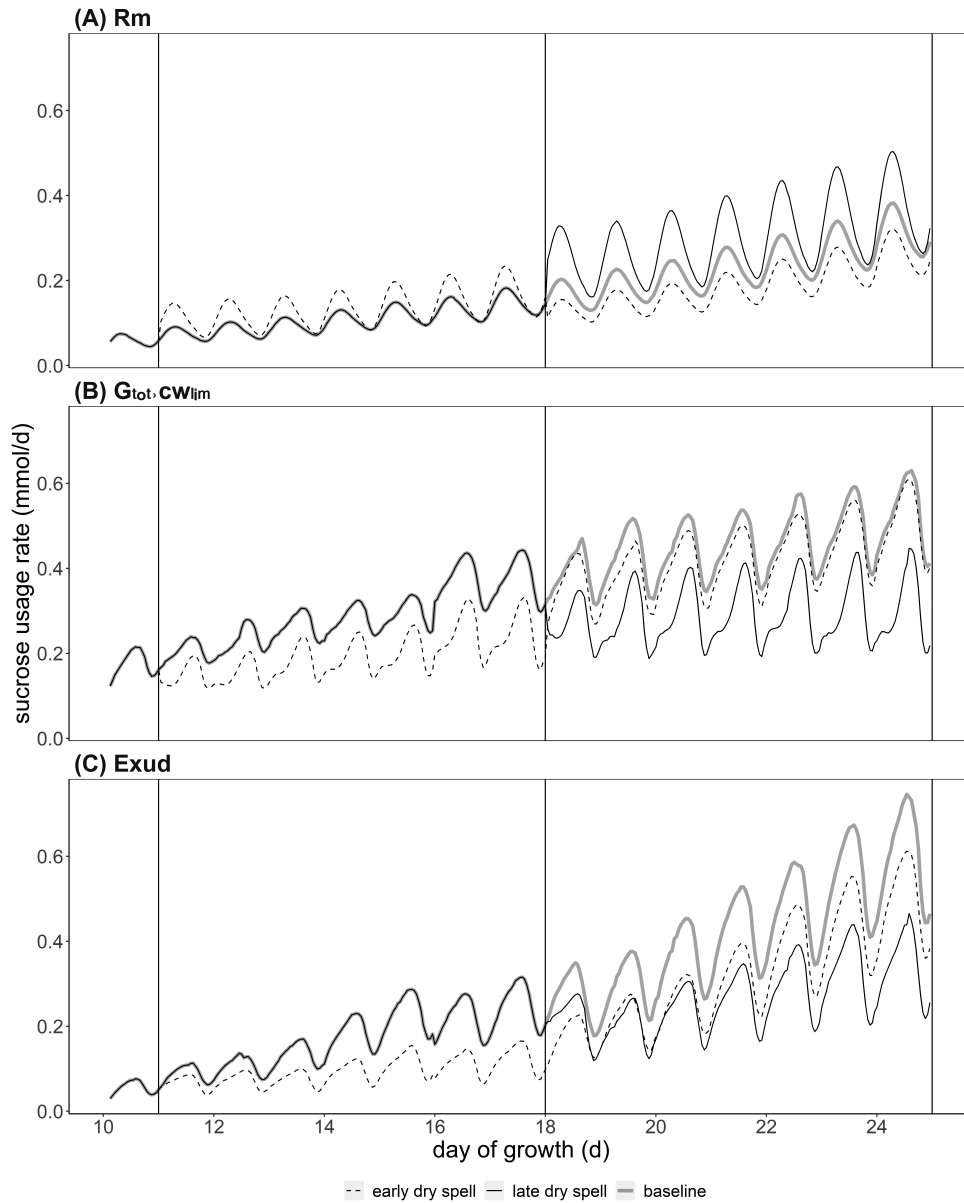


Figure 9. Partitioning of the carbon loss between the three sinks according to time: maintenance respiration (R_m), growth and growth respiration ($G_{\text{tot}, \text{CWlim}}$), root exudation ($Exud$). The black vertical lines define the start and end of the atmospheric dry spells (11–18 days or 18–25 days). We compare an early (thin dashed lines) and late dry spells (thin lines) against a baseline scenario (thick lines).

3.2. Sucrose usage and non-structural sucrose content

Figure 9 presents the sucrose partitioning between the different sinks. Figure H1 in Appendix H presents the same data but over a shorter period to give a clearer example of the daily s_{st} variations. During the dry spells, the absolute value of maintenance respiration (R_m) was higher because of the higher temperature, leading to a higher enzyme activity. The daily R_m peak was likewise caused by the higher temperature at midday.

Because of the sink prioritization (maintenance > growth), in case of low assimilation (night time) or high R_m (midday), growth respiration ($G_{\text{tot}, \text{CWlim}}$) diminished to fulfill the R_m need.

The minimum soil matrix potential ($\psi_{m, \text{soil}}$) remained constant at -129 hPa for baseline and outside of the dry spell periods.

At the beginning of the dry spells (11 or 18 days) minimum $\psi_{m, \text{soil}}$ ($\psi_{m, \text{soil}}$ in the upper soil layer) was -467 hPa. At the end of the dry spell simulations (18 or 25 days), minimum $\psi_{m, \text{soil}} = -1376$ hPa for early dry spell and -1984 hPa for late dry spell. $\psi_{m, \text{soil}}$ and h_{atm} affected the symplast turgor potential ($\psi_{p, \text{symplast}}$): the minimum $\psi_{p, \text{symplast}}$ was 8537 hPa for baseline, 7119 hPa for early dry spell and 8095 hPa for late dry spell. For early dry spell, $\psi_{p, \text{symplast}}$ was closer to the critical symplast turgor potential for growth below which no growth occurs ($\psi_{p, \text{crit}, 2}$, set to 2000 hPa), leading to a lower $G_{\text{tot}, \text{CWlim}}$. Soil and air water contents had, therefore, a moderate effect on $G_{\text{tot}, \text{CWlim}}$.

$Exud$ varied according to s_{st} and was lower at night time. Moreover, we saw similar variations of $Exud$ during the dry

spells. Indeed, The higher R_m and the lower assimilation rate (see Fig. 14) for *early dry spell* and *late dry spell* were not compensated by the decrease in $G_{\text{tot,CWlim}}$ and led to a lower daily maximum $Exud$ when compared with *baseline*.

Table 3 gives the absolute values of the cumulative R_m , $G_{\text{tot,CWlim}}$, and $Exud$ at the end of the simulations. Compared with *baseline*, *early dry spell* and *late dry spell* led to a strong decrease of cumulative $G_{\text{tot,CWlim}}$ (-17% and -21% respectively), and $Exud$ (-30% and -26% , respectively). *early dry spell* led to a slight decrease of cumulative R_m (-5%) while *late dry spell* led to a strong increase of cumulative R_m ($+20\%$).

Figure 10 presents the mean s_{st} per organ type. s_{st} did not vary strongly during the simulation: it always remained between $0.42 \text{ mmol cm}^{-3}$ and $0.82 \text{ mmol cm}^{-3}$. For this simulation, the

Table 3. Total value of the cumulative sucrose sinks at the end of the simulation in mmol for maintenance respiration (R_m), growth and growth respiration ($G_{\text{tot,CWlim}}$), root exudation ($Exud$).

Scenario	R_m	$G_{\text{tot,CWlim}}$	$Exud$
<i>baseline</i>	2.44	5.37	4.23
<i>early dry spell</i>	2.30	4.47	2.97
<i>late dry spell</i>	2.93	4.22	3.14

starch dynamic in the sieve tube was dependent on the gradient between s_{st} and $s_{\text{targ,st}}$. As we set $s_{\text{targ,st}} = 0.4 \text{ mmol cm}^{-3}$, the starch reserves of the plant only increased during the simulation. During the dry spells the lower assimilation rate and higher R_m

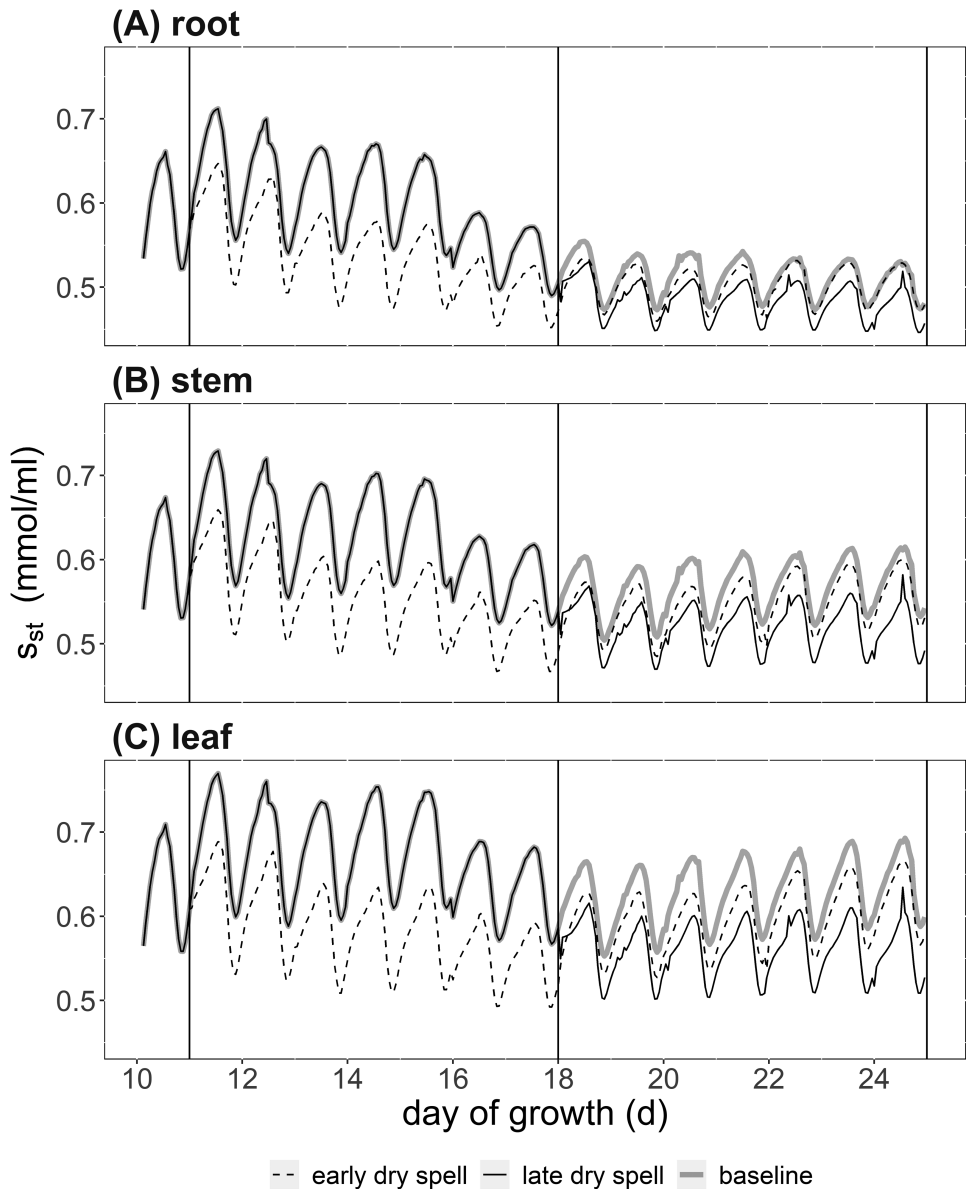


Figure 10. Mean sucrose concentration (s_{st}) according to time in the (A) root, (B) stem and (C) leaf organs. The black vertical lines define the start and end of the dry spells (11d to 18 days or 18–25 days). We compare an early (thin dashed lines) and late dry spells (thin lines) against a baseline scenario (thick lines).

led to a lower s_{st} compared with *baseline*. For *early dry spell*, the difference in s_{st} was maintained even after the end of the dry spell. These differences in s_{st} in the roots caused the different *Exud* observed in Fig. 9.

3.3. Structural sucrose content

Figure 11 presents the absolute structural sucrose content for each organ type and subtype.

At the beginning of the dry spell (11d, resp. 18 days), the monocots under *early dry spell* (resp. *late dry spell*) and *baseline* were exactly identical. We can observe several growth

plateaus in the development of the stems. This was caused by the user-defined growth delay of the main stem and tillers. It was used to represent the period after the first appearance of the stem and before the stem elongation phase.

Moreover, the lower $G_{tot,CWlim}$ under *early* and *late dry spell* (see Fig. 9) led to a lower growth for all organ types. Especially, we see a lower growth for *late dry spell* compared with *baseline*, which fits with the lower $G_{tot,CWlim}$ observed in Fig. 9. For all simulation scenarios, we can observe that the growth rate of the second-order laterals is much higher after Day 18.

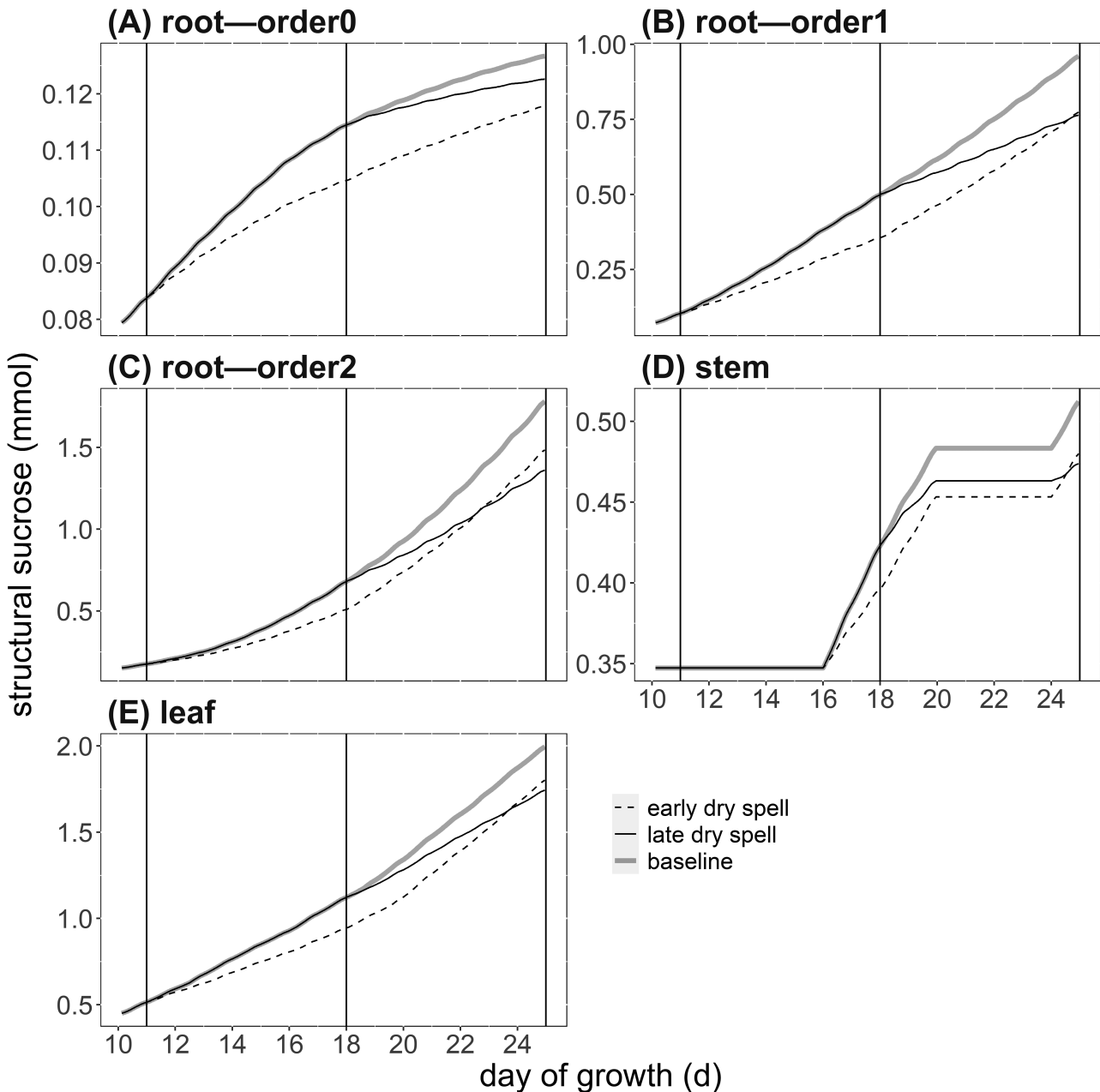


Figure 11. Absolute structural sucrose content per plant organ type and subtype according to time, with (A) 0-order roots; (B) first-order roots, (C) second-order roots, (D) stem (E) and leaf organs. Structural sucrose corresponds to the carbon in the plant tissues, in equivalent sucrose. The black vertical lines define the start and end of the dry spells (11–18 days or 18–25 days). We compare an early (thin dashed lines) and late dry spells (thin lines) against a baseline scenario (thick lines).

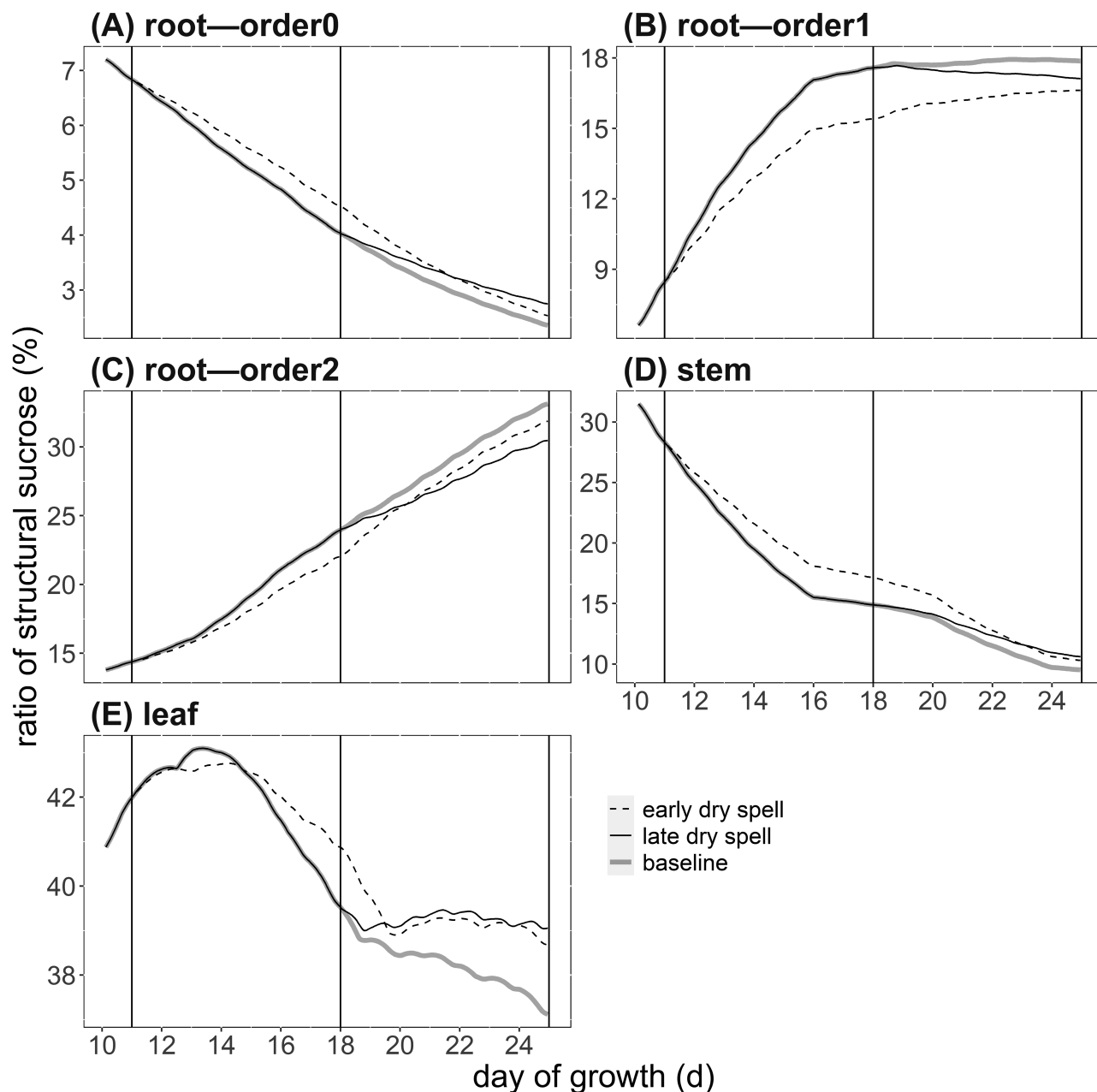


Figure 12. Relative structural sucrose content per plant organ type and sub-type according to time, with (A) zero-order roots; (B) first-order roots, (C) second-order roots, (D) stem (E) and leaf organs. Structural sucrose corresponds to the carbon in the plant tissues, in equivalent sucrose. The black vertical lines define the start and end of the dry spells (11–18 days or 18–25 days). We compare an early (thin dashed lines) and late dry spells (thin lines) against against a baseline scenario (thick lines).

Figure 12 presents the relative structural sucrose content for each organ type and sub-type.

For all simulations, the root-to-shoot ratio of structural sucrose content increased during the simulation. We observed that the dry spell intensities had a slight effect on the relative structural sucrose partitioning.

For instance, the final relative sucrose content in the root was 53% for *baseline*, 51% for *early dry spell* and 50% for *late dry spell*.

Because the growth of the second-order roots was much more important after Day 18, *late dry spell* had the lowest relative

structural sucrose content of second-order roots (30%) when compared with *baseline* (33%).

Figure 13 shows the 3D representation of the plants at the end of the simulation. Under *baseline* (13A), we observed a higher development of the leaves and root systems compared to *early dry spell* and *late dry spell* (13B and 13C). Indeed, the lower increase in root structural carbon is reflected by the different total root lengths per root order at Day 25: we obtained 3456 cm for *baseline*, 2793 cm for *early dry spell* and 2586 cm for *late dry spell*.

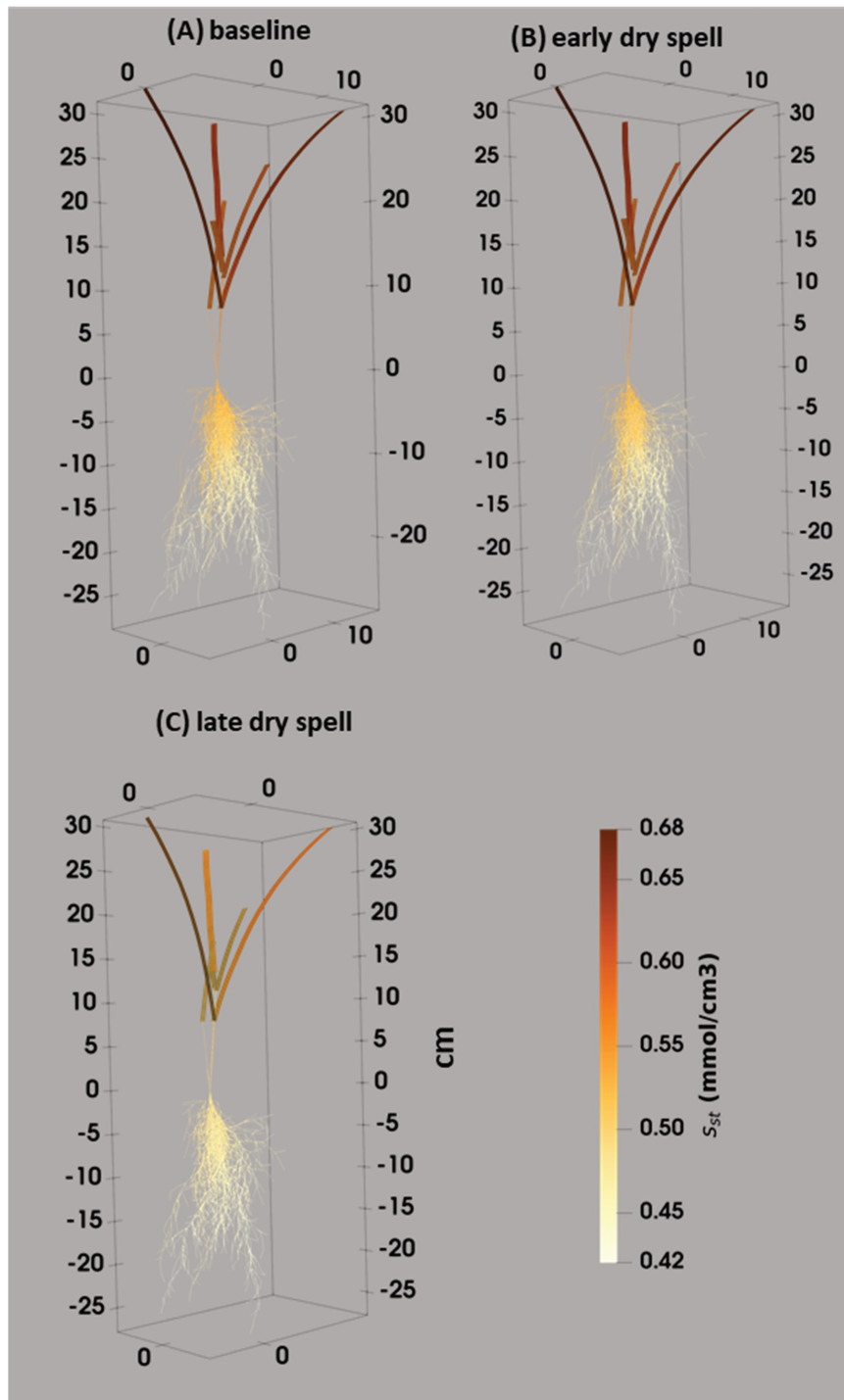


Figure 13. 3D representation of the virtual plants at 25 days after (A) baseline wetter and colder scenario, or drier and warmer dry spells (B) between Days 11 and 18, (C) between Days 18 and 25. Each segment is coloured according to its sucrose concentration in the sieve tube (s_{st} , mmol cm^{-3}).

Likewise, we can observe the different total leaf length per plant at Day 25: we obtained 161 cm for *baseline*, 148 cm for *early dry spell* and 145 cm for *late dry spell*.

Moreover, Fig. 13 allows us to see the s_{st} gradient along the plant's organs. For instance, longer mature leaves had the highest s_{st} values.

Finally, we could observe that the root system of *late dry spell* is less fibrous than under *baseline*, as observed in section

3.3. This was linked to lower development of the higher-order roots.

3.4. Instantaneous water-use efficiency

Figure 14 presents the cumulative transpiration and sucrose assimilation (cumulative $A_{g, \text{plant}}$, in mmol) for all scenarios (*baseline*, *early dry spell* and *late dry spell*).

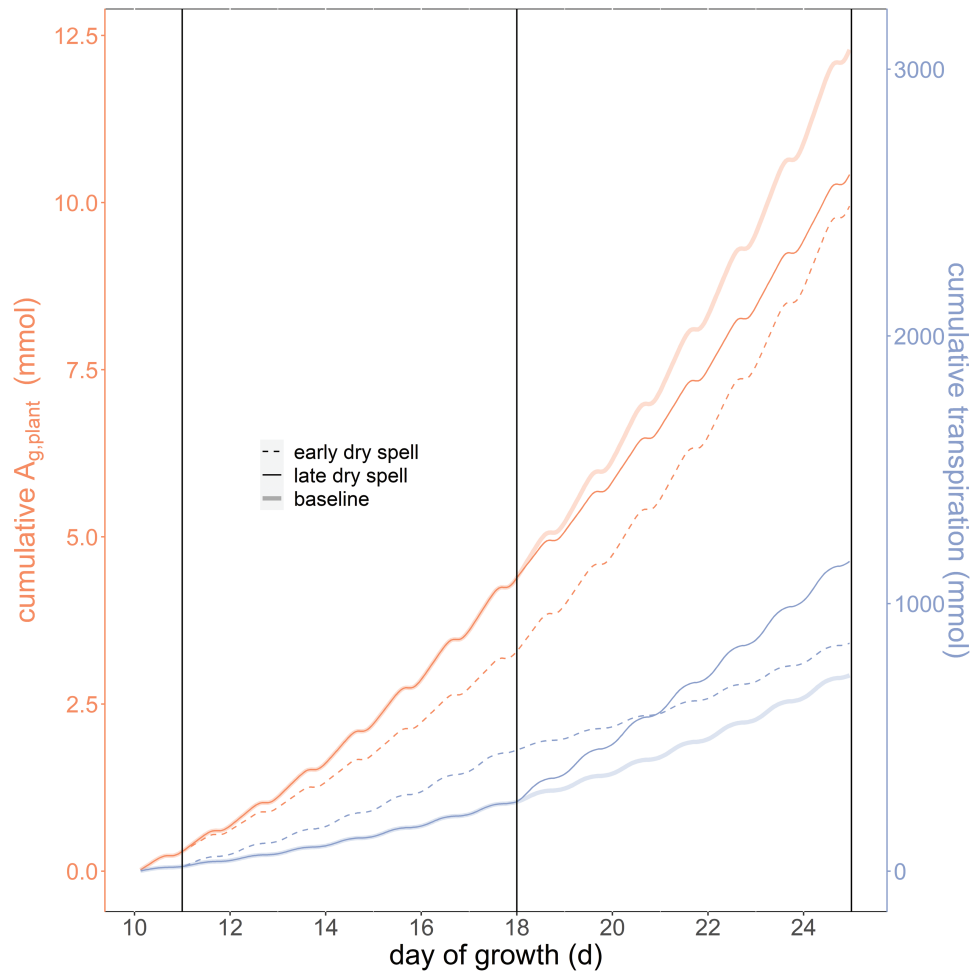


Figure 14. Cumulative assimilation of sucrose ($A_{g,plant}$, in orange) and cumulative transpiration (blue) according to time. The black vertical lines define the start and end of the dry spells (11–18 days or 18–25 days). We compare an early (thin dashed lines) and late dry spells (thin lines) against a baseline scenario (thick lines).

The dry spells had a negative effect on cumulative $A_{g,plant}$: -19% for *early dry spell* and -15% for *late dry spell*, when compared with *baseline*. This is caused by the lower leaf development (see Section 3.3) and by the lower assimilation rate per unit of leaf area (A_g).

For all simulations, we observed a small closing of the stomata because of the leaf water potential near midday. The water scarcity factor for stomatal opening (f_{w1}) went down to 0.94 for *baseline* scenarios, 0.86 for *early dry spell* and 0.91 for *late dry spell*. A smaller opening of the stomata led to a lower substomatal CO_2 concentration (c_i) and through this also caused the lower A_g for *drier&warmer*. Likewise, for *early dry spell* and *late dry spell*, maximum air temperatures of 303.42 K, above the optimum value of 298.15 K, led to a lower A_g .

Moreover, the higher leaf to air vapour pressure deficit during the dry spells led to a higher cumulative transpiration compared with *baseline*: $+16\%$ for *early dry spell* and $+58\%$ for *late dry spell*.

Overall, we observed a decrease in instantaneous water-use efficiency ($A_{g,plant}$ -to-transpiration ratio) at the end of the simulation for the dry spells scenarios compared with *baseline*: -30% for *early dry spell* and -46% for *late dry spell*.

4. DISCUSSION

4.1. CPlantBox offers a user-friendly flexible representation of the interactions between plant development and water and carbon fluxes

In this model, we implemented modules that were already included in other FSPMs: 3D representation of shoots and roots (Seleznova and Hanan 2018; Zhou et al. 2020), linked carbon and water fluxes (Seleznova and Hanan 2018; Zhou et al. 2020; Lacoite and Peter E. H. Minchin 2019), carbon respiration (Barillot, Chambon, and Andrieu 2016; Gauthier et al. 2020), exudation (Zhou et al. 2020), distributed carbon sources, sinks and storage (Lacoite and Peter E. H. Minchin 2019), water and/or carbon dependent growth (Postma et al. 2017; Coussement et al. 2020; Louarn and Song 2020; Gauthier et al. 2020), coupled soil and root water flux (Khare et al. 2022), effects of the atmosphere variables and plant water status on the coupled stomatal opening and photosynthesis (Tuzet, Perrier, and Leuning 2003). The novel aspect of this latest implementation of CPlantBox comes from linking all of these modules within one single user-friendly framework (Louarn and Song

2020) to represent the carbon and water fluxes in the soil–plant–atmosphere continuum. This allowed us to look at the feedback effects between plant growth and water and carbon fluxes, which were lacking in earlier models (Damour et al. 2010; Soualiou et al. 2021; De Swaef et al. 2022; Zhou et al. 2020). Processes that are usually predefined in FSPMs, like carbon partitioning (Postma et al. 2017; Soualiou et al. 2021), became consequently emerging properties of our model. We could, therefore, simulate how growth and carbon partitioning vary according to the growth conditions via semi-mechanistic process descriptions.

CPlantBox is also a flexible model: the spatial and temporal resolution (respectively, plant segment length and time step) can be defined at run time by the user. CPlantBox can also represent a wide variety of plants, contrary to other available FPSMs (Coussement et al. 2020; Louarn and Song 2020).

This is in agreement with the aims of CPlantBox which is to be a tool to (i) test the effect of the interactions between plant genotype, environmental conditions and agricultural management; (ii) help understand how/why these interactions lead to emerging properties (like plant structure and photosynthetic capacity); and (iii) return output parameters used as inputs by crop models (like carbon partitioning).

On the computing side, CPlantBox represents organisms using a graph formalism (similarly to OpenSimRoot (Postma et al. 2017)). This representation allows us to implement existing solvers created for graphs or 1D meshes (Hindmarsh et al. 2005; Guennebaud, Jacob, et al. 2010; Koch et al. 2021). These solvers greatly increase the efficiency of the flow computation (Lacointe and Peter E. H. Minchin 2019). Likewise, the implementation of CPlantBox in C++ with Python binding allows us to use the rapidity of C++ and the flexibility and clarity of Python. This is a non-negligible advantage as computational power becomes a significant limitation for the development of FSPMs (Soualiou et al. 2021; Coussement et al. 2020).

4.2. Results of the simulation

In this study, we used our model to look at the effect of a dry and warm spell of 1 week on plant water flow, carbon flow and growth, based on the expected temperature, air-relative humidity and relative variation in soil water content in Germany for June of 2100 (but without changes of CO₂ concentrations).

We could observe a lower growth rate for all organs, fitting with the results of X. Chen et al. (2021) for monocots under drought stress. In this simulation, the moderately lower turgor pressure during the drought affected the growth negatively. However, the lower growth was mainly caused by a lack of sucrose. This is contrary to the literature consensus as water stress is linked to a higher sucrose concentration because the lower growth rate over-compensates the lower assimilation (Lemoine et al. 2013; Michelena and John S. Boyer 1982). This change in osmotic potential leads in turn to a higher turgor pressure in the symplast (Lemoine et al. 2013; Michelena and John S. Boyer 1982). The effect of the water stress on the plant's sucrose concentration can, however, be adapted by recalibrating the phloem module. Moreover, the coupling between the sucrose concentration and symplast turgor pressure can be represented by implementing the symplast pressure and solution flow of PiafMunch (Lacointe and Peter E. H. Minchin 2019).

We observed a lower assimilation-to-transpiration ratio during and after the dry spells compared with the baseline. This was also observed experimentally by Tshikunde et al. (2018) for a monocot. The influence of the leaf area on the plant's photosynthetic capacities confirms the assumption of Damour et al. (2010) in their review of stomatal regulation models.

During the simulation, the ratio of exudation to total carbon usage remained within the range found in the literature for monocots: 3–40% (Dilkes, D. L. Jones, and Farrar 2004). However, as soil-soluble carbon concentration was a constant during the simulation, we could not model the feedback effects of different exudation levels. The plant sucrose concentration varied between 0.4 and 0.9 mmol cm⁻³, which fits with the values reported by (M. Thompson and N. Holbrook 2003; Jensen, Savage, and N. Michele Holbrook 2013). The low pressure gradient between source and sinks follows as well the current assumption for herbaceous angiosperms (De Schepper et al. 2013).

Contrary to other modelling studies, the dry spells did not lead to a decrease in transpiration (Tuzet, Perrier, and Leuning 2003; Bingham and Wu 2011). Indeed, the slight closing of the stomata did not compensate the higher evaporative demand caused by the lower air relative humidity. Additionally, the initial soil water potential remained high. The chosen grid resolution for the soil (1 cm³) was also relatively coarse and might have led to an over-estimation of the plant water uptake and thus of the transpiration (Khare et al. 2022). As shown by Khare et al. (2022), representing rhizosphere drying helps simulate more accurately the flow of soil water and root water uptake under dry conditions. A module representing this process is currently available within CPlantBox, but was not used within this study. Moreover, we did not represent the loss of conductivity caused by cavitation and this process can strongly affect the transpiration rate (Corso et al. 2020; De Swaef et al. 2022). Likewise, we did not simulate the stomatal closure linked to an increase in s_{meso} (De Schepper et al. 2013), which would have led to a lower assimilation and transpiration for the plants at the beginning of the simulation, when s_{st} is higher. Divergences between our model and other observed or simulated results remain, however, useful as they can give insight into which processes are key to representing emerging properties.

4.3. Current limitations of the model and future perspectives

The increasing number of modules in CPlantBox leads to a high number of parameters and (intermediary) outputs. Also, several variables and parameters cannot be measured experimentally (like the separation of the respiration between maintenance and growth (John H. M. Thornley 2011)) making their experimental evaluation more complex.

A first sensitivity analysis (Appendix G) was, therefore, done to evaluate the most important parameters. Moreover, several controls were set up in CPlantBox to warn the user in case of impossible outputs (like negative transpiration rate and too high sucrose concentration in the sieve tube). Building on this work, the development of an effective calibration pipeline and parameter database would be an important step towards making this model more readily usable (Louarn and Song 2020). On the experimental side, new (field) experiments will be conducted to

parameterize the model for a specific wheat genotype rather than a generic C3 monocot. When CPlantBox is not precisely parameterized, it can be used to do qualitative tests rather than quantitative predictions. Until the new modules are calibrated and tested against real data, this new version of CPlantBox should, moreover, be used to do qualitative evaluations rather than quantitative predictions.

The fixed-point approach used for the plant water flow–photosynthesis–stomatal regulation modules (Sections 2.1.4 and 2.1.4) always converged for our simulations (convergence reached in < 5000 loops). However, in case of a slow convergence (small variable variation between two consecutive loops), the computation time might become very high or the software might assume prematurely convergence. Adapting the computation scheme would make flow–photosynthesis–stomatal regulation modules more robust to a wide range of set-up. Moreover, the other modules are solved sequentially. Therefore, the selected time step needs to be small enough to avoid divergence. In the future, other parts of the module coupling which are more susceptible to diverge (like the coupled plant–soil water flow) will be solved with an implicit time stepping.

Regarding the functional processes represented, the accuracy of the phloem flow outputs could be further improved by adapting the representation of the sucrose usage. First of all, the plant's respiration is currently following the widely used growth-maintenance paradigm. As other processes/functional modules are added into CPlantBox (like nitrogen uptake and flow), it will be possible to shift to a process-based definition of the respiration rate, as recommended by Cannell and J. H. M. Thornley (2000) and implemented by Gauthier et al. (2020). This would also improve the evaluation of the feedbacks between the environmental conditions and the plant's processes. Also, the representation of the sucrose exudation rate, and of the chlorophyll-dependent assimilation offers the first elements of a more explicit representation of the nutrient flow within the plant, which are an important aspect of a plant's adaptation to its environment (Galindo-Castañeda et al. 2022). Moreover, the representation of sucrose-induced closing of the stomata would help evaluate the plant's sucrose-related adaptation capacity to a changing environment (De Schepper et al. 2013). The negative feedback of the sucrose on photosynthesis would, on the other hand, help better represent the decrease of photosynthetic capacity in case of low sucrose usage. Representing tissue death caused by water and/or carbon scarcity would allow CPlantBox to simulate plant development under more extreme weather conditions.

It would, moreover, be possible to update the internal CPlantBox–PiafMunch module to represent other processes available in PiafMunch, such as the osmotic and elastic adjustments of the plant tissues to its water content. Integrating these processes would allow us to simulate more precisely possible compensation between the total and osmotic potential in the symplast in case of drought (Michelena and John S. Boyer 1982). While elastic deformation of the xylem (Corso et al. 2020) and phloem (M. V. Thompson 2006) was not found to have a strong effect on their respective conductivities, elastic adjustment of the symplast can, however, lead to a higher resilience to droughts by maintaining a higher water potential in the plant (shrinking) (Kramer and Boyer 1995) or by increasing its water storage capacity (expansion) (Saliendra and Meinzer 1991).

Moreover, water stress can lead to a lower growth even when turgor pressure and sucrose concentration are high Michelena and John S. Boyer (1982), via, for instance, phytohormones, which we cannot yet represent in CPlantBox.

Regarding the 3D representation of the plant, the first description of graminaceous shoot growth was implemented: the leaf sheaths grow together upward, making a pseudo stem. We have, moreover, a stem elongation phase. The user can then set up an age-dependent tropism function to have the bending of the leaf blade once they have reached a specific age. The explicit 3D representation of the shoot organs makes it possible to simulate precisely the atmospheric variables (like PAR , T , g_{bb} , g_{canopy}) for each leaf segment. Next implementations of the model could include the simulations of the canopy micro-climate.

5. CONCLUSION

In this paper, we presented the latest version of CPlantBox and implemented it to represent the effect of atmospheric dry spells of 1 week, starting at different days (11 against 18 days after sowing) and compared the results with a baseline wetter and colder scenario. We could observe that the dry spells led to lower growth and exudation rates. The model also showed that the early dry spell affected the plant processes (higher transpiration, lower assimilation and lower organ growth) less than the late dry spell when compared with the wetter and colder climate.

The model was, therefore, capable of computing plant variables at a sub-diurnal scale and for each plant control volume in a complex architecture (fully grown monocot with distributed water and carbon sink and sources). The model could, moreover, simulate semi-mechanistically the interplay between the 3D plant topology and the environmental conditions via the water and carbon flows in the soil–plant–atmosphere continuum by representing a growing plant in a dynamic environment. The computed variables at small time and spatial scales led to emerging properties that are usually less precisely defined in plant models (growth rate and carbon partitioning).

CPlantBox is a versatile open-source tool that can be used to test hypotheses and understand the underlying relations between selected processes leading to specific phenotypes under different genotype–environment–management combinations.

Next steps in the development of CPlantBox will include the set-up of a calibration pipeline and the gathering of field and laboratory data to represent a specific plant phenotype, in order to test the model's capacity to mimic experimental outputs.

SUPPORTING INFORMATION

The following additional information is available in the online version of this article –

Table S1. Soil parameters.

Table S2. Notation, symbols, values (std) and units—input parameters of the structural CPlantBox modules.

Table S3. Notation, symbols, values and units—input parameters of the functional CPlantBox modules.

Table S4. Xylem tubes' shapes.

Table S5. Sieve tubes' shapes.

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CONTRIBUTIONS BY THE AUTHORS

S.L.G., Y.R. and M.G. conceived the experiments. S.L.G. and M.H. ran the experiments under the supervision of Y.R. and D.v.D. M.G. implemented the model changes described in Appendix A under the supervision of A.S., G.L., D.L. and J.V. S.L.G. and M.G. calibrated the model. M.G. ran the simulations under the supervision of A.S. and G.L. D.L., A.S., F.M. and M.J. set up the equations (and wrote) Part I.2.2 and Appendix H.2.1. S.L. wrote Appendix G.1. M.G. wrote the other parts of the manuscript under the supervision of AS and GL. All authors provided critical feedback and helped shape the research, analysis and manuscript.

CONFLICT OF INTEREST STATEMENT

None declared

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MODEL AVAILABILITY

The CPlantBox code used to run the simulations is available at <https://github.com/Plant-Root-Soil-Interactions-Modelling/CPlantBox/releases/tag/v2.0>. All the files used to run the simulations and plot the results are also available on Zenodo: [10.5281/zenodo.8106144](https://doi.org/10.5281/zenodo.8106144).

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APPENDICES

A. WATER POTENTIALS, CONDUCTIVITIES, AND CONDUCTANCES

We evaluate the water potentials in four domains: the soil, the xylem, the sieve tubes and the atmosphere, respectively, denoted with the subscripts *soil*, *x*, *st* and *atm*. For clarity, we define here the total potential ψ_t and its components in each of those domains. We define ψ_t as

$$\psi_t = \frac{\eta - \eta_{\text{ref}}}{\bar{V}} = \psi_p + \psi_g + \psi_o,$$

where η and η_{ref} are the chemical potentials of the considered and reference water, respectively, ψ_p is the pressure potential, ψ_g is the gravitational potential and ψ_o is the osmotic potential (Nobel 2009b). ψ_p includes all the potentials except the osmotic and gravitational ones and can be positive (absolute $\psi_p > \text{absolute } \psi_{p,\text{ref}}$) or negative (absolute $\psi_p < \text{absolute } \psi_{p,\text{ref}}$). In unsaturated soils,

$$\psi_{p,\text{soil}} = \psi_{m,\text{soil}} + \psi_{a,\text{soil}} < 0$$

with ψ_m the matric potential and ψ_a the pneumatic potential. The pneumatic potential corresponds to the over-pressure of the

Table A1. Notation, symbols and units - variables and other parameters

Symbol	Description	Units
Photosynthesis		
A_g	gross carbon assimilation rate per unit of surface	$\text{mmol cm}^{-2} \text{ day}^{-1}$
$A_{g,q}$	daily gross carbon assimilation	mmol day^{-1}
c_i	substomatal CO_2 molar fraction	$\text{mmol}^{-1} \text{ mmol}^{-1}$
c_{atm}	CO_2 molar fraction at the site of measurement	$\text{mmol}^{-1} \text{ mmol}^{-1}$
D	vapor deficit coefficient	—
E_v	water vapor flow rate per leaf area	$\text{cm}^3 \text{ cm}^{-2} \text{ day}^{-1}$
ea	actual vapor pressure	hPa
es	saturated vapor pressure	hPa
f_{w1}	water scarcity factor of the stomatal model	—
g_{CO_2}	conductance to CO_2	$\text{mmol cm}^{-2} \text{ day}^{-1}$
g_{HO_2}	conductance to HO_2	$\text{mmol cm}^{-2} \text{ day}^{-1}$
h	relative humidity	—
Je	electron transport rate for a set for a set <i>PAR</i>	$\text{mmol cm}^{-2} \text{ day}^{-1}$

Table A1. Continued

Symbol	Description	Units
$J_{e_{\max}}$	maximal electron transport rate	$\text{mmol cm}^{-2} \text{ day}^{-1}$
$J_{e_{\max}}^{25}$	maximal electron transport rate at 25°C	$\text{mmol cm}^{-2} \text{ day}^{-1}$
M_{CO_2}	Michaelis coefficient for CO_2	mmol mmol^{-1}
M_{O_2}	Michaelis coefficient for O_2	mmol mmol^{-1}
P_{atm}	atmospheric air pressure	hPa
PAR	photosynthetic active radiation	
	absorbed by the plant	$\text{mmol photons cm}^{-2} \text{ day}^{-1}$
R_d	dark respiration rate	$\text{mmol cm}^{-2} \text{ day}^{-1}$
Res	resistivity	$\text{d cm}^2 \text{ cm}^{-3}$
F_c	carboxylation rate	$\text{mmol cm}^{-2} \text{ day}^{-1}$
F_{cmax}	maximal carboxylation rate	$\text{mmol cm}^{-2} \text{ day}^{-1}$
F_{cmax}^{25}	maximal carboxylation rate at 25°C	$\text{mmol cm}^{-2} \text{ day}^{-1}$
V_j	electron transport rate	$\text{mmol cm}^{-2} \text{ day}^{-1}$
Γ	CO_2 compensation point	mmol mmol^{-1}
Γ^*	CO_2 compensation point in the absence of mitochondrial respiration	mmol mmol^{-1}
Other		
a	element's radius or leaf thickness	cm
A_{cross}	cross-sectional area	cm^2
$Exud$	sucrose sink for exudation	mmol day^{-1}
$[Exud]$	sucrose sink for exudation	$\text{mmol cm}^{-3} \text{ day}^{-1}$
$F_{in}, F_{out}, F_{out,MM}$	source terms for s_{st} loading, total unloading, and unloading with Michaelis-Menten	mmol day^{-1}
$[F_{in}], [F_{out}], [F_{out,MM}]$	source terms for s_{st} loading, total unloading, and unloading with Michaelis-Menten	$\text{mmol cm}^{-3} \text{ day}^{-1}$
G_{tot}	sucrose sink for growth	mmol day^{-1}
$[G_{\text{tot}}]$	sucrose sink for growth	$\text{mmol cm}^{-3} \text{ day}^{-1}$
j_{lat}	solution lateral flux	$\text{cm}^1 \text{ day}^{-1}$
J	solution volumetric flow rate	$\text{cm}^3 \text{ day}^{-1}$
K_{ax}	intrinsic axial conductance for the solution	$\text{cm}^4 \text{ hPa}^{-1} \text{ day}^{-1}$
k_{lat}	area specific conductance of the membrane	$\text{cm hPa}^{-1} \text{ day}^{-1}$
L, l	total length, arbitrary small length	cm
p	perimeter	cm
r	growth rate	cm day^{-1}
R_m	sucrose sink for maintenance	mmol day^{-1}
$[R_m]$	sucrose sink for maintenance	$\text{mmol cm}^{-3} \text{ day}^{-1}$
$s, \bar{s}$	sucrose concentration, residual between actual and minimum sucrose concentration	mmol cm^{-3}
s_q	sucrose content	mmol
$starch$	starch concentration	mmol cm^{-3}
t	time	d
v	volume	cm^3
W	leaf blade's or sheath's width	cm
T	temperature	K
z	height, $z = 0$ at the soil surface, upward-pointing axis	cm
μ	dynamic viscosity	hPa d
ξ	local axial coordinate of the plant	cm
ψ	water potential	hPa
$\Omega, \partial\Omega$	studied domain and its boundaries	—
Subindices		
0	initial or residual value	
<i>atm</i>	atmosphere	
<i>ax</i>	axial	
<i>bl</i>	leaf boundary layer	
<i>blade</i>	leaf blade	
<i>canopy</i>	canopy	
<i>Clim</i>	carbon limited	
<i>CWlim</i>	carbon and water limited	
<i>crit</i>	critical	
<i>h</i>	hydrostatic (in phloem: turgor)	

Table A1. Continued

Symbol	Description	Units
Subindices		
g	gravitational	
i, j	plant node index	
in	entering the sieve tube	
l	value over the length l	
lat	lateral	
lim	limited	
m	matric potential	
max	maximum (potential) value	
$meso$	mesophyll	
o	osmotic potential	
ox	outer xylem	
org	organ	
out	outside of plant (value) or leaving the plant (flow)	
p	turgor pressure (in xylem: hydraustatic potential)	
$sheath$	leaf sheath	
ref	reference	
$sheath$	leaf sheath	
$soil$	soil	
seg	plant segment (discretised model) studied plant zone (continuous model)	
st	phloem sieve tube	
$stomata$	stomata	
t	total	
x	xylem	
$wlim$	water limited	

Table A2. Number of samples per parameter for each simulation for the Sobol sensitivity analysis

scenario \ plant age	water modules		carbon modules	
	11 day	18 day	11 day	18 day
baseline	2 ¹²	2 ¹²	2 ¹¹	2 ¹¹
dry spell	2 ¹²	2 ¹²	2 ¹¹	2 ¹¹

air: $\psi_a = P_{atm} - P_{soil\ air} \cdot P_{atm}$ (hPa) is the atmospheric pressure at ground level, dependent on the pressure of all the gases in the Earth's atmosphere. The reference water (denoted with the subscripts ref) is pure, at ground level ($z_{ref} = 0$), and the hydrostatic potential equals the atmospheric pressure. In the plant, $\psi_p = \psi_h$, with ψ_h the hydrostatic potential. ψ_p is generally positive in the plant tissues and is also called the turgor pressure. For specific cells, like the xylem $\psi_{p,x}$ is usually under tension. All the water potentials are given in hPa (corresponding to $100 \times \text{Joule}/\text{m}^3$).

In this paper, the flow of fluids considered can be computed with either the lateral conductivity ($k_{lat,Y}$, in $\text{L P}^{-1}\text{T}^{-1}$, here in $\text{cm hPa}^{-1} \text{day}^{-1}$), or the intrinsic axial conductance ($K_{ax,Y}$, in $\text{L}^4\text{P}^{-1}\text{T}^{-1}$, here in $\text{cm}^4 \text{hPa}^{-1} \text{day}^{-1}$) (Meunier et al. 2017). lat stands for lateral and ax for axial. Y is a stand in for the denomination of the flow channel (compartment, tissue, membrane, etc.) considered.

For the photosynthesis module, we use the stomatal conductance in molar units ($g_{Z,Y}$, in $\text{N L}^{-2}\text{T}^{-1}$, here in $\text{mmol cm}^{-2} \text{day}^{-1}$), with Z standing in for either H_2O or CO_2 .

For the soil module, the hydraulic conductivity (κ_{soil}), units are in $\text{cm}^2 \text{hPa}^{-1} \text{day}^{-1}$ ($\text{L}^2 \text{P}^{-1}\text{T}^{-1}$) given the definition of the soil water potential.

B. COMPUTATION OF THE PLANT SHAPE VARIABLE

An organ's length is equal to the sum of the length of its segments: $L_{seg} \leq L_{org}$, with L in cm. Root and stem organs are defined as cylinders, where shapes are computed from their lengths and radii (a in cm). In the current CPlantBox implementation, a is constant for all segments of the organ: $a_{seg} = a_{org}$.

Leaf organs are defined as cuboids where shapes are computed from their thicknesses (a in cm) and widths (w in cm). The leaf organs are separated in two regions: the sheath and the blade. a and w of the sheath can be different to that of the blade.

The seed is represented by one node linking the main stem (and tillers) with the zero-order roots. The sieve tubes and xylem tissues are defined as cylinders. Each organ can have one or more sieve tube or xylem cylinders. Finally, the shape of the mesophyll is assumed to be equal to that of the leaf blade it is in (for instance, with v , the volume in cm^3 : $v_{meso} = v_{blade}$).

A_{cross} (cross-sectional area, cm^2), v (volume, cm^3) and p (perimeter of the exchange surface, cm) of all the organs, segments, sieve tubes and xylem tissues are calculated thus:

$$v_Y = \begin{cases} v_{sheath} + v_{blade} & \text{for leaf organs} \\ A_{cross,Y} \times L_Y & \text{else} \end{cases} \quad (B1)$$

$$A_{cross,Y} = \sum_i^{n_X} A_{cross,Y,i} \quad (B2)$$

$$p_Y = \sum_i^{n_X} p_{Y,i} \quad (B3)$$

$$A_{cross,Y,i} = \begin{cases} w_Y a_Y & \text{for leaf blades and sheaths} \\ \pi a_{Y,i}^2 & \text{else} \end{cases} \quad (B4)$$

$$p_{Y,i} = \begin{cases} 2w_i & \text{for leaf blades and sheaths} \\ 2\pi a_{Y,i} & \text{else} \end{cases} \quad (B5)$$

with Y as a stand-in for either st (sieve tube tissues), x (xylem tissues), seg (segment), org (organ), $sheath$ (leaf sheath), and $blade$ (leaf blade). i represent one cylinder of the tissue type in the studied segment. n_Y corresponds to the number of tissue unit of segment (or vessel) per cross section of segment. Thus $n_{seg} = 1$. In our parameterized model, n_{st} (resp. n_x) corresponds to the number of vascular bundles per cross section times the number of sieve (resp. xylem) tubes of a specific radius per bundle. As p corresponds to the perimeter of the lateral exchange surface, we only take into account the width of the leaf and not its thickness, as, for our virtual plant, the stomatas are located on the upper and lower sides of the leaf blade.

C. PHOTOSYNTHESIS: AUXILIARY EQUATIONS

We present the below complementary equations that are used in the photosynthesis module.

C.1. Raoult's law

The area-specific water vapour flow rate $j_{lat,ox-atm}$ ($\text{cm}^3 \text{ cm}^{-2} \text{ day}^{-1}$) can be driven by the gradient of water vapour pressure (ea in hPa) or of total water potential (ψ_t in hPa). We convert ψ_t to ea using Raoult's law (Nobel 2009b):

$$\psi_{t,Y} = \frac{RT_Y \rho_{H_2O}}{Mm_{H_2O}} \ln \left(\frac{ea_Y}{es(T_Y)} \right) + \psi_{g,Y} \quad (C6)$$

with, for the domain Y , Mm_{H_2O} (kg mmol^{-1}) and ρ_{H_2O} (kg cm^{-3}), respectively, the water molar mass and density, $es(T_Y)$ (hPa) the saturation vapour pressure at temperature T_Y (K), the ideal gas constant R ($\text{cm}^3 \text{ hPa K}^{-1} \text{ mmol}^{-1}$) and the gravitational potential $\psi_{g,x}$ (hPa).

C.2. Plant functions

Several photosynthesis variables are dependent on the temperature. This temperature dependence can be described by the Arrhenius and the temperature inhibition functions (Bonan 2019): The Arrhenius function (Bonan 2019):

$$\text{Arrhenius}(T_{seg}, E_{a,X}) = \exp \left(\frac{E_{a,X}}{0.1 \times RT_{25}} \left(1 - \frac{T_{25}}{T_{seg}} \right) \right) \quad (C7)$$

$$\text{TempInhib}(T_{seg}, E_{d,X}) = \frac{1}{1 + \exp \left(\frac{ST_{seg} - E_{d,X}}{0.1 \times RT_{seg}} \right)} \quad (C8)$$

with $E_{a,j}$ and $E_{d,j}$ (mJ mmol^{-1}), respectively, the activation and deactivation energy. S ($\text{mJ mmol}^{-1} \text{ K}^{-1}$) is an entropy term. The factor 0.1 is used to go from hPa $\text{cm}^3 \text{ K}^{-1} \text{ mmol}^{-1}$ to $\text{mJ K}^{-1} \text{ mmol}^{-1}$.

M_{CO_2} , M_{O_2} , R_d , and Γ^* can be calculated with the following equation:

$$X_x = X_x^{25} \times \text{Arrhenius}(T_{seg}, E_{a,x}) \quad (C9)$$

where $E_{a,x}$ is the activation energy for X_x (either M_{CO_2} , M_{O_2} , R_d , or Γ^*) in mJ mmol^{-1} , and X_x^{25} is the value of X_x for $T = 298.15 \text{ K}$.

C.3. Air conductance

We separate the area outside the leaf in three zones: the laminar layer directly outside the leaf (boundary layer), the turbulent layer between the leaf boundary layer and the canopy-induced zero displacement height, the turbulent layer between the canopy-induced zero displacement height and the point of measurement. The effect of each layer is represented by a resistivity to the water vapour flow, respectively: $Res_{H_2O,bl}$, $Res_{H_2O,canopy}$, and $Res_{H_2O,atm}$, all in day cm^{-1} .

$Res_{H_2O,atm}$ is computed according to Allen et al. (1998):

$$Res_{atm,H_2O} = \frac{\ln \left[\frac{z_m - \frac{2}{3}h_p}{0.123 \times h_p} \right] \times \ln \left[\frac{z_m - \frac{2}{3}h_p}{0.1 \times h_p} \right]}{k_{Karman}^2 u_z} \quad (C10)$$

with z_m (cm) height of wind and humidity measurements, h_p (cm) the height of the highest plant node, k_{Karman} (0.41–) the von Karman's constant, u_z (cm day^{-1}) wind speed at height $z_m - \frac{2}{3}h_p$ is the canopy-induced zero displacement height.

We set the mean canopy resistance as (Nobel 2009d):

$$Res_{H_2O,canopy} = \frac{\frac{1}{3}h_p}{k_{eddy,canopy}} \quad (C11)$$

with $\frac{1}{3}h_p$ the mean length of the canopy turbulent layer between the leaf boundary layer and the canopy-induced zero displacement height, $k_{eddy,canopy}$ ($8.64e8 \text{ cm}^2 \text{ day}^{-1}$) the mean eddy covariance value, corresponding to the value given by Nobel (2009d) for the space 1 m below the top of a maize canopy. And, assuming a constant leaf boundary layer thickness of 0.03 cm, we obtain

$$Res_{H_2O,bl} = \frac{0.03}{Diff_{H_2O}} = 1.5e - 6$$

with $Diff_{H_2O} \approx 2e3 \text{ cm}^2 \text{ day}^{-1}$, the diffusion coefficient of water vapour in air (Nobel 2009c).

We can then convert the physical conductances ($\frac{1}{Res_{H_2O,Y}}$ in $\text{day cm}^1 \text{ cm}^{-2}$) in molar conductances ($g_{H_2O,Y}$ in $\text{mmol cm}^{-2} \text{ day}^{-1}$) (Nobel 2009c; Tuzet, Perrier, and Leuning 2003):

$$g_{H_2O,Y} = \frac{P_{atm}}{Res_{H_2O,Y} \times RT_Y} \quad (C12)$$

D. ASSUMPTION OF LOCAL WATER EQUILIBRIUM

M. Thompson and N. Holbrook (2003) presented a mathematical model to justify the assumption of water equilibrium between the xylem and the phloem. Briefly, when their $\hat{R}\hat{F}$ coefficient is above unity, equilibrium can be assumed.

In their model, they looked at a sieve tube with a constant radius and viscosity, where the loading and unloading of sucrose occurred at the boundaries. Those simplifications can be applied to our model when focusing on the segment level. Indeed, the (un)loading of sucrose occurs in the nodes at the segments' extremities. The $\hat{R}\hat{F}$ coefficient can be computed thus:

$$\hat{R}\hat{F}_{ij} = \frac{p_{st}}{A_{cross,st}} \times R T_{seg} s_{st,.} \times \frac{l_{seg}}{j_{ij}} \times k_{lat,st-x,w} \quad (D13)$$

$$s_{st,.} = \begin{cases} s_{st,j} & \text{if } j_{ij} \geq 0 \\ s_{st,i} & \text{else} \end{cases} \quad (D14)$$

with $k_{lat,st-x,w}$ the water permeability of the membrane linking the xylem and phloem tissues.

In order to have $\hat{R}\hat{F} \geq 1$, we had to adapt our parameter set to have $Fu = 0 \text{ mmol ml}^{-1} \text{ day}^{-1}$ (no usage of carbon) when $s_{st} < 0.4 \text{ mmol ml}^{-1}$. This fits with observations for wheat plant where s_{st} was observed to be above this value (M. Thompson and N. Holbrook 2003). For our four simulations, after a burn-in time of 3 h, we needed to have an area-specific conductance between the xylem and the phloem $k_{lat,st-x,w}$ at least equal to $1.1e - 4 \text{ cm day}^{-1} \text{ hPa}^{-1}$ so that $\hat{R}\hat{F} \geq 1$ for all segments. This value was found to be plausible for wheat plants. This confirms the analysis of M. Thompson and N. Holbrook (2003): in their study, they found this simplification to be acceptable for the transport system of most plants, including wheat.

Likewise, in the study of Lacoite and P. P. Minchin (2008) for $s_{st} > 0.15 \text{ mmol cm}^{-3}$, decreasing the permeability of the membrane between the xylem and phloem had no effect on the outputs.

The assumption of local water equilibrium between xylem and phloem was also tested in experimental studies and found to be acceptable (Sevanto, Hoelttae, and N. M. Holbrook 2011; Cabrita 2011, Section 2.2.1.5).

E. CALIBRATION AND NOTATIONS

E.1. Experiments for direct calibration

E.1.1. Plant growth conditions

The wheat phenotype studied in this experiment (UQR15) was obtained from the Hickey lab (University of Queensland, Australia) (Rambla et al. 2022). Thirteen PVC columns (diameter = 8 cm, height = 45 cm) were filled with silty loam soil from one testing site of the Research Center Jülich, located in Selhausen (50.8659 N, 6.4471 E). The columns received two seeds each (equivalent to a sowing density of 400 seeds/m²) and were afterwards installed in a climate chamber (20°C day, 18°C night, 50% RH, 1000 $\mu \text{mol m}^{-2} \text{s}^{-1}$ of PAR from 6 am to 8 pm). The mean initial soil gravimetric water content (θ_{soil}) was of $0.40 \text{ cm}^3 \text{ cm}^{-3}$. Water was added twice a week to keep the θ_{soil} value between 0.30 and $0.44 \text{ cm}^3 \text{ cm}^{-3}$.

Fertilizer (7% nitrate, 19% ammonium) was added at 6 and 34 days after sowing (stage Z11 and Z25 of the Zadok's growth scale, respectively) in liquid solution supplied at a rate of 3 kg m^{-2} .

E.1.2. Non-destructive measurements

The plant development was evaluated 2–3 times a week via the following measurements: number of tillers and leaves, plant stage (on the Zadok scale), and length and width of the leaves' blade. The chlorophyll content of the lowest and second highest leaf of each plant tiller was also recorded using a chlorophyll meter (SPAD502, Konika Minolta, Bremen, Germany). The mean θ_{soil} value for each column was measured by weighing the column on a scale.

E.1.3. Soil Water Profiler

In order to measure the transpiration rate, we used the Soil Water Profiler (SWaP) developed by Dusschoten et al. (2020). At 4, 5 and 6 weeks after sowing (stages Z24, Z25 and Z33, respectively), four of the soil columns were randomly selected. The measurements lasted 36 h (2-day and 1-night periods). The sensor temporal and spatial (vertical) resolutions were 15 min and 1 cm, respectively. The day-light intensity alternated between high and low irradiation levels every 4 h. The variation in total θ_{soil} allowed us to measure the root water uptake rate (assumed equal to the transpiration) at those irradiation levels. The soil surface was covered and the evaporation was thus assumed to be negligible. The same transpiration measurements were done while progressively increasing the irradiation level in order to measure the light saturation point.

E.1.4. Destructive measurement

Following the SWaP measurements, we extracted the root systems from the soil. The fresh weight of the roots, stems and leaves was measured. The roots were then stored in 30% ethanol solutions. The fresh weight of the root, stems and leaf was measured via a weighing scale (precision = 1 mg; Kern 572-30, Kern & Sohn GmbH, Balingen, Germany). The stems and leaves were stored in a freezer at -20°C . Afterwards, the leaves were scanned (Canon, 4 Krefeld, Germany) for analysis with ImageJ (Schindelin et al. 2012) to measure the leaf blade and sheath surface together with the position and number of the nodes along the stems. The volume of the leaves and stems was obtained by immersing them in a graduated cylinder containing water and measuring the variation of the water level. Lateral cuts of the leaf blades (at 5 cm to the leaf sheath, on the second leaf of the tiller), stems (at 1 cm above the soil, when the stems were present) and roots (at 9–18 cm depth) were done with a cryomicrotome (CM 3050S; Leica Microsystems GmbH, Wetzlar, Germany). The images were analysed with ImageJ to measure the number of vascular bundles and the average shape of the xylem and phloem tissues in each bundle.

E.2. Input parameters and other variables and parameters

Tables S1–S5 and Table A1 present the input parameters and variables of the model. The source used for the parameter estimation can be either (i) direct calibration—direct experimental measurements (see section above), (ii) indirect calibration—value set to fit with objective outputs, (iii) from the literature (copying the value or recomputing it from the dataset of the

publication), in which case the reference is given. The shoot shape parameters were obtained from the experiments described above while the root shape parameters (except for the phloem and xylem tissues) were taken from Bingham and Wu (2011), as adapted by Schnepf et al. (2018).

F. NUMERICAL SOLUTION

In this section, we first give an overview of the main notations used to describe the numerical solutions. We then define the analytical solution for the xylem water flow, leaf outer-xylem water flow (transpiration) and phloem flow for one segment. Finally, we describe the matrix notation and solving scheme. Numerical details of the soil water flow are described in Koch et al. (2021).

F.1. Mathematical definitions

The branched plant structure is divided into connected line segments with N_s segments and N_n nodes. From the point of view of a mathematical graph, it corresponds to a directed tree (see Section 2.1.2). According to the graph (or mesh) terminology, a CPlantBox node is a graph node (mesh vertex) and a CPlantBox segment is a graph edge (mesh cell). For the definition of segment or node variables: We define the segment ij as the segment going from i to j .

We have for the segment flows: $J_{ij} = -J_{ji}$. For other segment variables, $X_{ij} = X_{ji}$. Subscripts of brackets or parenthesis ($[\dots]_{ij}$, $(\dots)_{ij}$) apply to all the variables within. For the definition of matrices, the subscript *seg* indicates vectors of size $[N_s, 1]$ containing segment data. *node* indicates vectors of size $[N_s + 1, 1]$ containing node data. The sign ‘ $\cdot$ ’ indicates a hadamard product, ‘ $\oslash$ ’ a hadamard division and T indicates a transposition.

The FvCB-stomatal regulation variables (such as A_g , $g_{CO_2, stomata}$, see Section 2.1.4), the xylem water-flux variables ($J_{ax,x}$, $J_{lat,x-soil}$, $J_{lat,x-atm}$, see Section 2.1.4) and the phloem solution axial flux ($J_{ax,st}$, see Section 2.1.4) are solved for each segment. The other sucrose-related variables (s_{st} , s_{meso} , F_{in} , F_{out} , see Sections 2.1.4, 2.1.4) and $\psi_{t,x}$ (see Section 2.1.4) are solved for each node.

IM is the incidence matrix of the directed graph (of size $[N_n, N_s]$) and IM^T is its transposition (of size $[N_s, N_n]$). Thus we have:

$$IM[j, k] = \begin{cases} -1 & \text{if a segment } k \text{ has } j \text{ as begin-node} \\ 1 & \text{if a segment } k \text{ has } j \text{ as end-node} \\ 0 & \text{else} \end{cases} \quad (F15)$$

BM is a boolean matrix of size $[N_s, N_n]$. It gives for each segment the index of the upflow node:

$$BM[k, j] = \begin{cases} 1 & \text{if } IM[j, k] \times J_{w, seg}[k] < 0 \\ 0 & \text{else} \end{cases} \quad (F16)$$

with $J_{w, seg}[k]$ the net water flow of the segment k going from the begin node to the end node. Therefore, $BM[k, j] = 1$ only if the water flow in the segment k goes from the node j to the other node of the segment k .

F.2. Analytical solution for one segment

In this following section, we present the definition of the driving equations of Sections 2.1.4, 2.1.4 and 2.1.4, discretized for one plant segment (graph edge) or node (graph vertex).

F.2.1. Plant water flow

F.2.1.1. Axial flow The analytical solution to Equation (31) presented below is based on the approach of Landsberg and Fowkes (1978) and Meunier et al. (2017, Appendix B). However, contrary to them, (i) we define the xylem axial flow according to $\psi_{p,x}$ and not $\psi_{t,x}$ (ii) we use an exponential function instead of an hyperbolic function.

When $k_{lat,x} > 0$ and $K_{ax,x} > 0$, we use the analytical continuous solution

$$\psi_{p,x}(l) = \psi_{out} + d_i e^{\tau l} + d_j e^{-\tau l} \quad (F17)$$

$$\psi_{out} = \begin{cases} \psi_{m, soil} & \text{if belowground} \\ \psi_{p, ox} & \text{if leaf} \end{cases} \quad (F18)$$

with ψ_{out} (hPa) the water potential outside of the plant, uniform over the axial distance l . The above equation is solved with

$$\tau = \sqrt{p_{org} \times k_{lat,x} / K_{ax,x}} \quad (F19)$$

where the constants d_i and d_j (hPa) can be calculated from the boundary conditions.

To discretize the equation for each segment ij , the Dirichlet top ($l = 0$), and bottom ($l = L$) boundary conditions are given by the begin and end nodes of the segment: $\psi_{p,x}(0) = \psi_{p,x,i}$ and $\psi_{p,x}(L) = \psi_{p,x,j}$. They are inserted into the analytic solution and yield the two equations

$$\begin{pmatrix} 1 & 1 \\ e^{\tau L} & e^{-\tau L} \end{pmatrix}_{ij} \begin{pmatrix} d_i \\ d_j \end{pmatrix}_{ij} = \begin{pmatrix} \psi_{p,x,i} - \psi_{out,ij} \\ \psi_{p,x,j} - \psi_{out,ij} \end{pmatrix}. \quad (F20)$$

Each plant segment is given a mean $\psi_{m, soil, ij}$ ($\psi_{m, soil, ij}$ of the voxel were the segment centre is located) or $\psi_{p, ox, ij}$. Therefore, $\psi_{out, ij}$ is a constant. From these equations, we can calculate the constants $d_{i, ij}$ and $d_{j, ij}$ of the segment ij as

$$\begin{pmatrix} d_i \\ d_j \end{pmatrix}_{ij} = \delta_{ij}^{-1} \begin{pmatrix} e^{-\tau L} & -1 \\ -e^{\tau L} & 1 \end{pmatrix}_{ij} \begin{pmatrix} \bar{\psi}_{p,i} \\ \bar{\psi}_{p,j} \end{pmatrix}_{ij} \quad (F21)$$

with

$$\delta_{ij} := [e^{-\tau L} - e^{\tau L}]_{ij}, \quad (F22)$$

and

$$\bar{\psi}_{p,i, ij} = \psi_{p,x,i} - \psi_{out, ij} \quad (F23)$$

$$\bar{\psi}_{p,j, ij} = \psi_{p,x,j} - \psi_{out, ij} \quad (F24)$$

Thus, $\bar{\psi}_{p,i, ij}$ and $\bar{\psi}_{p,j, ij}$ are constants.

Putting the constants $d_{i, ij}$ and $d_{j, ij}$ into the solution for $\psi_{p,x}$ (Equation (F17)), we can write down the exact axial flow in the segment ij , as (Meunier et al. 2017, B2):

$$J_{ax,x, ij}(l) = -[K_{ax,x} (d_i \tau e^{\tau l} - d_j \tau e^{-\tau l} + d \psi_g(l))]_{ij} \quad (F25)$$

with $d\psi_g(l)$ the gradient of gravitational water potential between the nodes i and the point at l cm from i . Replacing the constants $d_{i,ij}$ and $d_{j,ij}$ with their definition yields the explicit axial flow equation:

$$J_{ax,x,ij}(l) = -K_{ax,x,ij} \left[\delta^{-1} \tau \left[(e^{-\tau l} \bar{\psi}_{p,x,i} - \bar{\psi}_{p,x,j}) e^{\tau l} - (-e^{\tau l} \bar{\psi}_{p,x,i} + \bar{\psi}_{p,x,j}) e^{-\tau l} \right] + d\psi_g(l) \right]_{ij} \quad (F26)$$

Evaluation of the axial flow at $l = 0$ (node i) yields

$$J_{ax,x,ij}(0) = -K_{ax,x,ij} \left(\delta^{-1} \tau \left[(e^{-\tau L} + e^{\tau L}) \bar{\psi}_{p,i} - 2\bar{\psi}_{p,j} \right] + d\psi_g(0) \right)_{ij}. \quad (F27)$$

For conservation of mass in each node i , the summed exact axial flows have to equal zero,

$$\sum_{j \in N(i)} J_{ax,x,ij}(0) = 0 \quad (F28)$$

where $N(i)$ are the indices of the segments starting from node index i to j . We can solve this system of equations (see [Appendix F.2.5](#)) and obtain thus $\psi_{p,x}$ and $J_{ax,x}$ for each plant node and segment, respectively.

$\psi_{p,x}$ and $J_{ax,x}$ are then used by the photosynthesis and phloem module ([Equations \(20\)](#) and [\(33\)](#)) and by the core CPlantBox module to compute the water-limited growth rate ([Equation \(2\)](#)).

F.2.1.2. Lateral flow Once $\psi_{p,x}$ is known, the exact lateral water flow ($J_{lat,x-out}$, in $\text{cm}^3 \text{day}^{-1}$) for a segment ij with length L_{ij} and lateral conductivity $k_{lat,x,ij}$ can be computed with the following equations:

$$J_{lat,x-out,ij} = -[p_{org} k_{lat,x}]_{ij} \int_0^{L_{ij}} \psi_{out,ij} - \psi_{p,x} dl \quad (F29)$$

$$J_{lat,x-out,ij} = \left[p_{org} k_{lat,x} \left(\frac{d_i}{\tau} (e^{\tau L} - 1) + \frac{d_j}{\tau} (1 - e^{-\tau L}) \right) \right]_{ij} \quad (F30)$$

Inserting the definition of $d_{i,ij}$ and $d_{j,ij}$ into the exact lateral flow yields

$$J_{lat,x-out,ij} = \left[p_{org} k_{lat,x} \frac{1}{\delta \tau} \times (\bar{\psi}_{p,i} (1 - e^{-\tau L} - e^{\tau L} + 1) + \bar{\psi}_{p,j} (-e^{\tau L} + 1 + 1 - e^{-\tau L})) \right]_{ij} \quad (F31)$$

and

$$J_{lat,x-out,ij} = \left[p_{org} k_{lat,x} \frac{1}{\delta \tau} (\bar{\psi}_{p,i} + \bar{\psi}_{p,j}) (2 - e^{-\tau L} - e^{\tau L}) \right]_{ij} \quad (F32)$$

The $J_{lat,x-out}$ values from root segments can then be used as source term in the soil module (see [Section 2.1.5](#)). The $J_{lat,x-out}$ values from leaf segments corresponds to the transpiration rate (see [Section 2.1.4](#)).

F.2.2. Stomatal regulation, photosynthesis, and transpiration

Once $\psi_{p,x}$ and $J_{lat,x-atm}$ are known, we can compute $\psi_{p,ox}$ (hPa), the water potential on the surface of the leaf vascular bundle sheath, by implementing [Equations \(F31\)](#), and solving for ψ_{out} (here, equivalent to $\psi_{p,ox}$):

$$\psi_{p,ox,ij} = \left(\left[\frac{J_{lat,x-atm} \times L \times p}{k_{lat,x} \frac{1}{\tau \delta} (2 - e^{-\tau L} - e^{\tau L})} \right]_{ij} + (\psi_{h,x,i} + \psi_{h,x,j}) \right) \times 0.5 \quad (F33)$$

$J_{lat,x-atm}$ is obtained from [Equation \(7\)](#). $\psi_{p,ox}$ can then be used in the xylem flow module (see [Equation \(30\)](#)) at the next computation loop.

F.2.3. Sucrose balance

As explained above, s_{st} , s_{meso} , F_{in} , F_{out} are node variables. When segment-defined variables or parameters are needed to compute them (such as v_{st} , A_g , $k_{lat,st}$), we allocate to the node i the variable from the segment i which has i as end node: $X_{i,node} = X_{i,seg}$.

We set $s_{Y,q}$ (mmol sucrose) the sucrose content in the compartment Y , either the mesophyll or the sieve tube.

$\frac{ds_{q,j}}{dt}$ (mmol sucrose day^{-1}), the variation of sucrose content in the node j , is defined thus:

$$\frac{ds_{st,q,j}}{dt} = J_{ax,st,q,j} + (F_{in,j} - F_{out,j}) \quad (F34)$$

$$J_{ax,st,q,j} = \sum_i^{N_n} (s_{ij} \times J_{ax,st,H_2O,ij}) \quad (F35)$$

$$J_{ax,st,H_2O,ij} = \frac{K_{ax,st,ij}}{L_{ij}} \times (RT \times (s_j - s_i) + (\psi_{xj} - \psi_{xi})) \quad (F36)$$

$$s_{ij} = \begin{cases} s_i, & \text{if } J_{w,ij} < 0 \\ s_j, & \text{if } J_{w,ij} \geq 0, \end{cases} \quad (F37)$$

$$\frac{ds_{meso,q,j}}{dt} = (F_{Ag,i} - F_{in,i}) \times v_{meso,i}. \quad (F38)$$

ψ_{xj} and ψ_{xi} are obtained, thanks to the xylem flow computation (see [Sections 2.1.4](#) and [F.2.1](#)). $F_{Ag,i}$ corresponds to the sucrose assimilation rate computed according to [Equations \(17\)](#), [\(41\)](#). $F_{in,i}$ and $F_{out,i}$ are computed according to [Equations \(43\)](#) and [\(52\)](#), respectively. $J_{ax,st,q,j}$ (resp. $J_{ax,st,H_2O,ij}$) corresponds to the axial flow in the sieve tube of sucrose content (resp. water) at node i .

F.2.4. Matrix form and solving scheme

In the following section, we present the discretized system of equations and the solving schemes to obtain $\psi_{p,x}$, $\frac{ds_{st,q,j}}{dt}$ and $\frac{ds_{meso,q,j}}{dt}$.

F.2.5. Xylem water flow

From Equations (F27–F28), we can construct a system of equations, that can be solved for $\psi_{p,x}$:

$$\psi_{h,x,node} = C^{-1} \times b_{node} \quad (F39)$$

With C and b_{node} matrices of size $[N_n, N_n]$ and $[N_n, 1]$, respectively. They are filled with zeros except at the following locations:

$$C[i, i] = C[i, i] + c_{i,ij} \quad (F40)$$

$$C[i, j] = 2[K_{ax,x} \delta^{-1} \tau]_{ij} \quad (F41)$$

$$b_{node}[i, 1] = b_{node}[i, 1] + [K_{ax,x} \times d\psi_g]_{ij} + (c_{i,ij} + C[i, j])\psi_{out,ij} \quad (F42)$$

$$c_{i,ij} = [K_{ax,x} \delta^{-1} \tau(e^{-\tau L} + e^{\tau L})]_{ij} \quad (F43)$$

for each segment ij going from node i to node j .

This system of equation is solved for the steady-state solution of $\psi_{p,x}$ with the sparse linear solver (SParseLU) of the C++ Eigen library (Guennebaud, Jacob, et al. 2010). The $\psi_{p,x}$ are then used to compute the variables from the FvCB-stomatal regulations module. The fixed point iteration between the computation continues until convergence.

F.2.6. Sucrose balance

The equations from Section F.2.3 can be set in matricial form:

$$\left[\frac{ds_{st,q}}{dt} \right]_{node} = IM \times (J_{w,seg} \cdot s_{st,seg}) + (F_{in,node} - F_{out,node}) \cdot v_{st,node} \quad (F44)$$

$$s_{st,seg} = BM \times s_{st,node} \quad (F45)$$

$$s_{st,node} = s_{st,q,node} \odot v_{st,node} \quad (F46)$$

$$J_{w,seg} = Co_{ax,st,seg} (IM^T \times RTs_{st,node} + IM^T \times \psi_{x,node}) \quad (F47)$$

$$\left[\frac{ds_{meso,q}}{dt} \right]_{node} = (F_{Ag,node} - F_{in,node}) \cdot v_{st,node} \quad (F48)$$

with $Co_{ax,st,seg}$ the vector defining the conductance ($\text{cm}^3 \text{hPa}^{-1} \text{day}^{-1}$) per sieve tube segment.

The system of equations is solved numerically using an implicit method: the value of $s_{q,node}^{m,n}$ (the vector containing the estimation m at time step n of s_q per node) is used to compute $\left[\frac{ds_q^{m,n}}{dt} \right]_{node}$. This value is sent to the implicit Sundials-CVODE solver (Hindmarsh et al. 2005) which then yields $s_{q,node}^{m+1,n}$. This loops continue until convergence is reached. The solver then moves on to the next time step.

G. SENSITIVITY ANALYSIS

The programme contains a high number of plant parameters which cannot be measured directly and which are highly correlated between them with regards to the outputs. Therefore, to have a better idea of which parameters need to be (re)calibrated in priority, a first sensitivity analysis was run for (i) the coupled

water flow and FvCB-stomatal regulations modules (water modules), (ii) the phloem flow and carbon usage modules (carbon modules). A sensitivity analysis of the root system parameters only can be found in the work of Morandage et al. (2022).

As the computation time of the full coupled simulation is too long to run a sensitivity analysis, we evaluated the effect of the water (resp. carbon) modules' parameters for one time step of 3 h. We, moreover, focused on a selected number of output variables of interest, namely (i) the total transpiration and gross assimilation rates for the water modules and (ii) carbon usage rate for growth ($G_{tot,CWlim}$) for the carbon modules.

This sensitivity analysis is limited to a short time span and evaluates each module separately. Nonetheless, water (resp. phloem) parameters that have a strong influence on the transpiration and assimilation rates (resp. growth rate) will also influence strongly the other modules on the long term. For this evaluation, we did not include plant parameters which could be considered as physical constants, like E_a and E_d , respectively, the activation and deactivation energy parameters used in the photosynthesis model.

Like for our example of simulation, we only represented a starch dynamic in the sieve tube (resp. mesophyll) dependent on the gradient between s_{st} (resp. s_{meso}) and the target value $s_{targ,st}$ ($s_{targ,meso}$). The starch-related parameters representing other dynamics (e.g. $F_{max,starch}$, $k_{hyd,starch}$) were set to 0. To diminish the number of parameters to evaluate, some were regrouped. Consequently, k_{chl} represents the influence of Chl , $kchl1$ and $kchl2$; k_{starch} represents the influence of the starch-related parameters; X_{root} represents the influence of the parameter X for all the root types. We only selected key structural parameters. Moreover, some pre-tests allowed us to take out of the analysis parameters which had a very limited effect on the outputs (like oi) to lower as well the number of parameters evaluated.

The sample range of each evaluated parameter was set to $[\frac{1}{2}, 2]$ of their value used in this study, except for the values of α and ω . For these two variables, ranges were set to make sure that a solution for Equation (14) could be found. We used $\Delta\psi_{o,symplast}$ as parameter (which corresponds to $\psi_{o,symplast} - \psi_{t,crit2}$) instead of $\psi_{o,symplast}$ to avoid ever having $|\psi_{o,symplast}| > |\psi_{t,crit2}|$ which would have led to computation errors.

Moreover, the first analysis showed that the environmental conditions and the plant's development stage influenced the sensitivity of the outputs to the parameters. Therefore, the analysis was run for each plant age at the beginning of the simulations (11 or 18 days) and each weather type (*baseline*, *dry spell*) using the environmental variables for noon.

The analysis was done with the SALib python module (Iwanaga, Usher, and Herman 2022). The number of samples was set according to the trade-off between precision gain and computation speed loss (see table A2). Therefore, the simulations using slower modules were run with a lower number of parameter samples.

Figure G1 presents the outputs of the analysis. The variation of the sensitivity index according to the plant and environment's characteristics indicate that such analysis could be necessary for each model setup. The difference in the width of the confidence intervals is in part linked to the different number of samples used for each analysis (see Table A2).

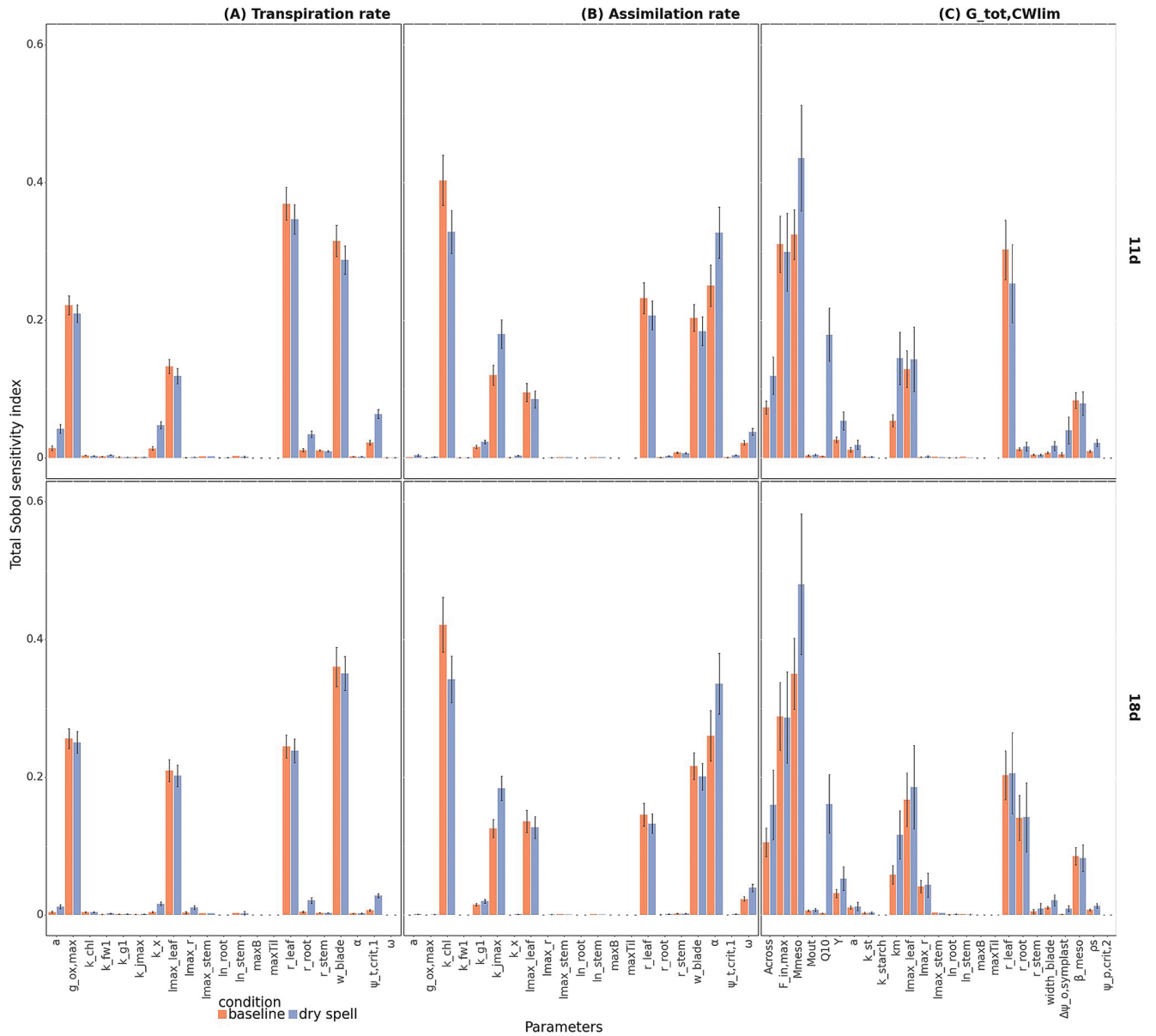


Figure G1. Sensitivity analysis of the plant's (A) transpiration and (B) gross assimilation rate to the water modules' parameter and (C) carbon usage rate for growth ($G_{\text{tot,CWlim}}$) to the carbon modules' parameters for 11 and 18 days plants under the two weather scenarios presented in the study. The sensitivity index includes both first-order effects and interactions with the other parameters. The error bars show the limits of the confidence interval (confidence level of 95%).

For the water modules, we can observe that $g_{H_2O,ox,max}$ is especially important. This parameter represents the conductivity between the leaf xylem bundle sheath and the substomatal cavity. Currently, $g_{H_2O,ox,max}$ is a set constant. The results indicate, therefore, that it is necessary to represent the variation of $g_{H_2O,ox,max}$ to evaluate more precisely the plant transpiration rate. For the assimilation rate, Chl (the leaf chlorophyll content), k_{chl1} and k_{chl2} (parameters linking the chlorophyll content to the potential assimilation rate), have a strong influence on the output of the simulation, because they affect the carboxylation rate (V_c). Similarly, α and k_{jmax} affects the photon-limited assimilation rate V_j . Moreover, the leaf structural parameters (l_{max} the maximum length, r_{leaf} the growth rate, w_{blade} the blade width) also had a strong

influence on the outputs, both the assimilation and the transpiration.

For the carbon modules, we can observe, for instance, that $G_{\text{tot,CWlim}}$ is especially sensible to the parameters defining the flow of sucrose from the mesophyll to the sieve tubes: $F_{in,max}$, M_{meso} and β_{meso} . This defines how quickly the assimilated sucrose flows in the sieve tube and has a strong influence on the plant's capacity to buffer changes in assimilation rate.

Surprisingly, $\psi_{p,crit,2}$ which defines the water limitation on growth, was found to have no influence on the outputs. It is likely caused by the fact that, for the simulated period, sucrose was more limiting than water for growth. Running a longer simulation for the sensitivity analysis should give a better evaluation of the influence of $\psi_{p,crit,2}$ on $G_{\text{tot,CWlim}}$.

H. OTHER SIMULATION RESULTS

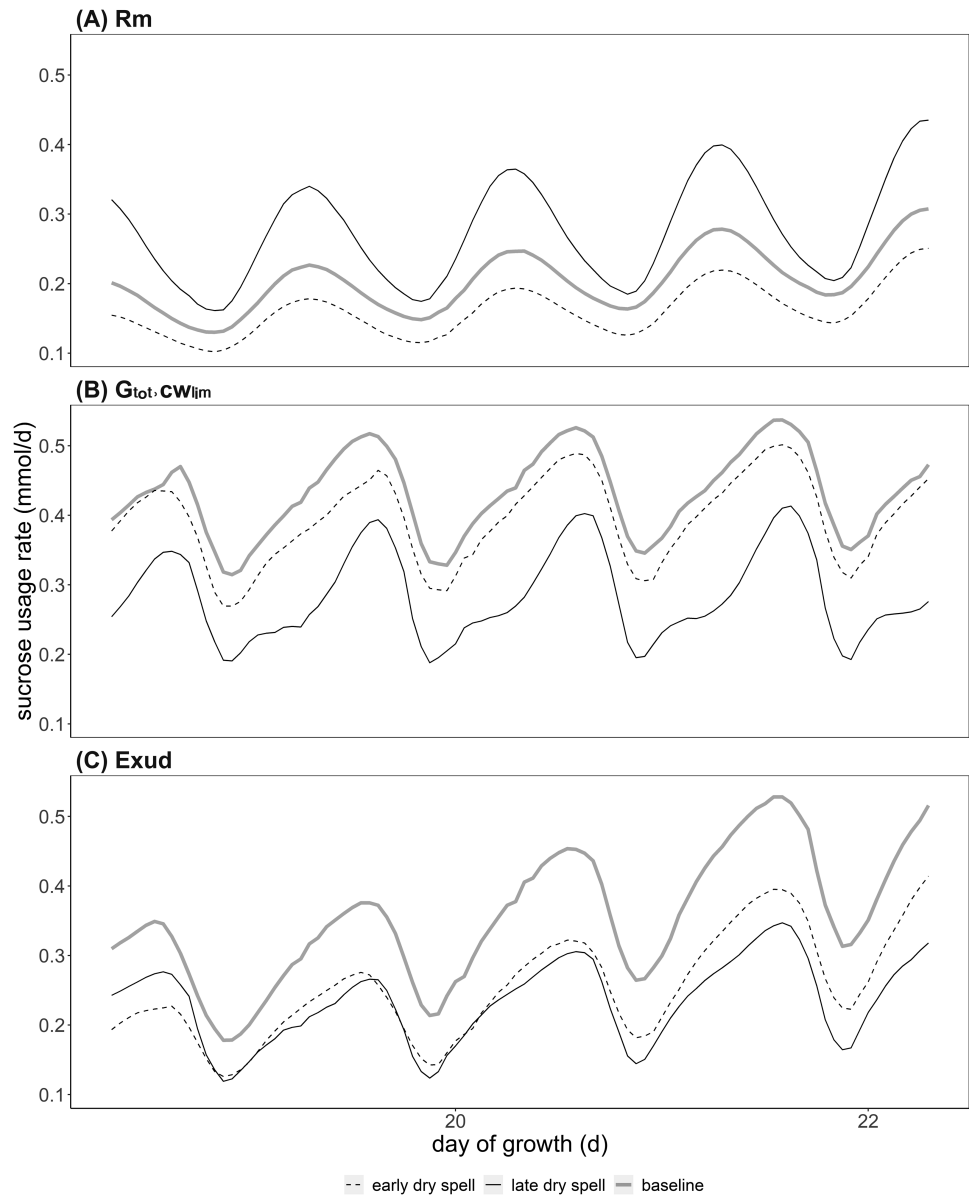


Figure H1. Partitioning of the carbon loss between the three sinks according to time between Days 19 and 23: maintenance respiration (R_m), growth and growth respiration ($G_{tot.CWlim}$), root exudation ($Exud$). We compare an early (thin dashed lines) and late dry spells (thin lines) against against a baseline scenario (thick lines).