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Original Research

CPlantBox, a whole-plant modelling framework for the simulation of water- and carbon-related processes

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ABSTRACT

The interaction between carbon and flows within the vasculature is at the centre of most growth and developmental processes. Understanding how these fluxes influence each other, and how they respond to heterogeneous environmental conditions, is important to answer diverse questions in agricultural and natural ecosystem sciences. However, due to the high complexity of the plant–environment system, specific tools are needed to perform such quantitative analyses. Here, we present CPlantBox, a whole-plant modelling framework based on the root system model CRootBox. CPlantBox is capable of simulating the growth and development of a variety of plant architectures (root and shoot). In addition, the flexibility of CPlantBox enables its coupling with external modelling tools. Here, we connected the model to an existing mechanistic model of water and carbon flows in the plant, PiafMunch. The usefulness of the CPlantBox modelling framework is exemplified in five case studies. Firstly, we illustrate the range of plant structures that can be simulated using CPlantBox. In the second example, we simulated diurnal carbon and water flows, which corroborates published experimental data. In the third case study, we simulated impacts of heterogeneous environment on carbon and water flows. Finally, we showed that our modelling framework can be used to fit phloem pressure and flow speed to (published) experimental data. The CPlantBox modelling framework is open source, highly accessible and flexible. Its aim is to provide a quantitative framework for the understanding of plant–environment interaction.

KEYWORDS: Architecture; Carbon; Model; Plant; Root; Shoot; Water.

INTRODUCTION

Plants contribute for ~80 % of the global earth biomass (Bar-On *et al.* 2018). They also strongly control land surface fluxes of water and carbon. Plant water uptake constitutes a major part of the evapotranspirative flux at the land surface but its prediction is extremely variable and uncertain (Trenberth *et al.* 2007; Jasechko *et al.* 2013; Vereecken *et al.* 2015). The same is true for the estimation of carbon-related fluxes (Metz *et al.* 2005; Ayllón *et al.* 2018). As such, understanding the interplay between plant carbon and water flows and their environment is of importance to answer diverse questions in agricultural and natural ecosystem sciences.

The flows of water and carbon in the plant are constrained by both local and global structures (Bidel *et al.* 2000; Draye *et al.* 2010; Fiorani and Schurr 2013; Lobet *et al.* 2013). Root architecture is known to have an impact on water uptake (Lynch 2013; Lobet *et al.* 2014a), while shoot structure has an impact on carbon assimilation through photosynthesis (Boardman 1977; Lichtenthaler *et al.* 1981; Zhu *et al.* 2010). From an entire plant perspective, root and shoot are tightly connected, forming a complex and dynamic continuum between water and carbon flows. For instance, water availability at the root level influences carbon status in the shoot, although the physiology behind this is unclear (Hummel *et al.* 2010; Fatichi *et al.* 2019). The stomata conductance directly affects root water uptake by changing xylem pressure (Tuzet *et al.* 2003; De Schepper and Steppe 2010). Knowing the connecting structure of both shoot and root is therefore needed to better understand plant water and carbon relations.

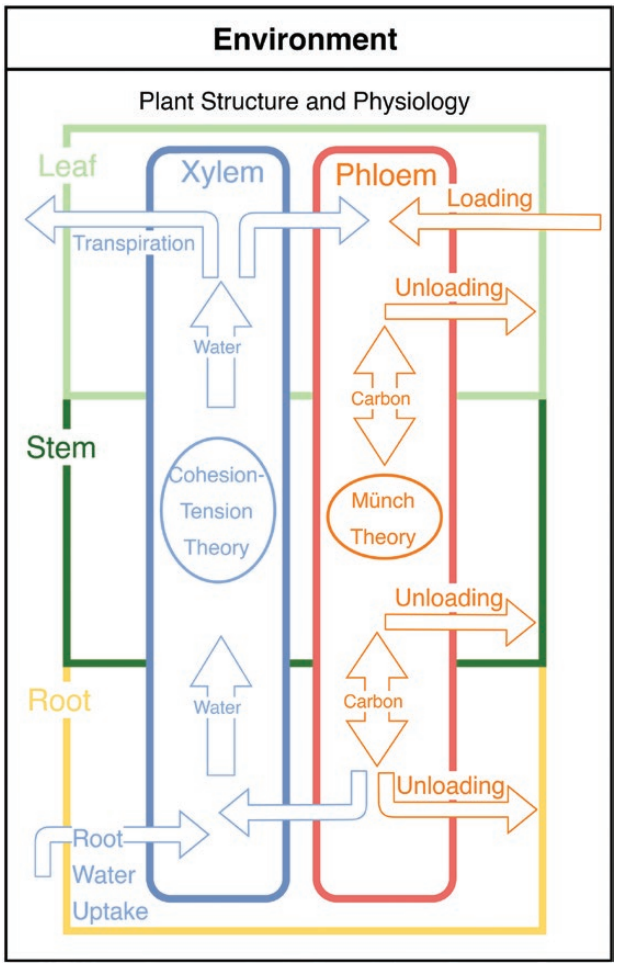

Figure 1. Structures and functions affect carbon and water flow in plants. Leaf and root contact the environment. Xylem and phloem connect organs and exchange carbon and water.

At the organ scale, the different parts of the plant (root, stem, leaves, flowers and fruits) are connected by the vasculature, which consist of xylem and phloem vessels (Fig. 1) (Jyske and Hölttä 2015; Savage *et al.* 2016). Xylem vessels transport the majority of water (Javaux *et al.* 2008; Schröder *et al.* 2008; Draye *et al.* 2010; Lobet *et al.* 2014), while phloem vessels translocate the majority of carbohydrates by pressure flow (Bidel *et al.* 2000; Van Bel 2003; Savage *et al.* 2013; De Swaef *et al.* 2015). The movement of water within the xylem vessels is typically explained by the tension–cohesion theory (Tyree 1997; Steudle 2001). This theory states that the transpiration at the leaf level creates a tension within the xylem vessels, which is transmitted to the soil–root interface and drives the water uptake from the soil. The carbon flow in the phloem continuum is explained by the Münch theory (Münch 1930; Knoblauch and Peters 2017). Briefly, Münch theory states that source organs (typically mature leaves and storage structures) load carbohydrates into the phloem sieve tubes. This strongly decreases the phloem solute water potential. Meanwhile, xylem and phloem vessels are tightly connected throughout the whole plant. This means the decreased osmotic potential in phloem will create a water flow from the xylem towards the phloem (Fig. 7C, light green line). This in turn increases water pressure in the phloem vessels, leading to a flow towards sink organs (typically roots, young leaves, flower and fruits) (roots are shown in Fig. 7C, light yellow line) (Jensen *et al.* 2012; Comtet *et al.* 2017). Recent experiments have provided the first direct support to the Münch theory by direct measurement (Knoblauch *et al.* 2016; Savage *et al.* 2017).

In recent years, new phenotyping techniques (Fiorani *et al.* 2012; Lobet and Draye 2013; Rellán-Álvarez *et al.* 2015, 2016; van Dusschoten *et al.* 2016; Marshall-Colon *et al.* 2017; Hui *et al.* 2018; Lobet *et al.* 2019) have enabled the precise measurements of plant structure with high temporal and spatial resolution. However, physiological parameters, such as pressure and flows in plants, are still challenging to measure. For example, the first pressure measurement in phloem sieve tubes was conducted only recently with a success rate lower than 30 % (Knoblauch *et al.* 2014, 2016). Another common issue with flow and pressure data is the fragmentation of the acquired data. In other words, data can only be acquired on specific organs and at specific times, which makes it difficult to structurally understand the underlying processes. More comprehensive and quantitative studies are therefore needed to better understand the complex dynamics between the water and carbon flow within the plant, in response to heterogeneous environments (Thompson and Wolniak 2008; Mullendore *et al.* 2010).

Recently, modelling tools have been proven very useful to study water and carbon flows in plants and to analyse environmental controls on these fluxes (Fatichi *et al.* 2019; Mencuccini *et al.* 2019). In particular, functional-structural plant models (FSPMs) have a long history of simulating water or carbon flows (De Reffye and Hu 2003; Kang *et al.* 2008; Pradal *et al.* 2008; Leitner *et al.* 2010; Vos *et al.* 2010; Xu *et al.* 2011; Lobet *et al.* 2014b; Sievänen *et al.* 2014; Zhu *et al.* 2016). Table 1 lists the most recent FSPMs simulating either the full plant structure (both root and shoot), or water and carbon flows. Among these, only a handful of 3D full plant structure models (with both 3D topology and 3D geometry) exist (Drouet and Pagès 2003; Janott *et al.* 2011; Lobet *et al.* 2012). Meanwhile, only two existing models were designed to simulate carbon and water flow simultaneously (Lacointe and Minchin 2008; Seleznyova and Hanan 2018).

We distinguish three approaches to model carbon distribution within the plant. The first approach prescribes allocation rules of assimilates between the different plant organs. The total pool of carbon is divided between different organs, which adjust their growth accordingly (Heuvelink 1996; Marcelis 1996). Usually, models using such approach do not need a fast computational method to distribute the carbon. A second approach uses detailed mechanistic relationships to simulate carbon (and sometimes water) flow within a simplified structure. These lumped models often only represent the plant as a small set of objects (Fig. 2B) (De Swaef *et al.* 2015; Steppe *et al.* 2015). Finally, a third approach resolves carbon and water flow within a 3D structure based on mechanistic relations between the different organs. Although these models (Bidel *et al.* 2000; Lacointe and Minchin 2008; Lopez *et al.* 2008; Seleznyova and Hanan 2018) can be computationally very intensive, they open the way to more complex representation of the plant–environment system.

Table 1. Overview of recent 3D topology and 3D geometry whole-plant (shoot and root) FSPMs.

Model name	Authors	Structure	Species	Flow(s)	Availability	Interface
GRAAL[a]	Drouet and Pagès (2003)	3D full plant	Maize	Water	–	GUI
PlaNet-Maize[a]	Lobet *et al.* (2012)	3D full plant	Maize	Water	Open source	GUI, Web interface
–[b]	Seleznyova and Hanan (2018)	3D full plant topology	Small plants	Water and carbon	–	–
L-Peach	Da Silva *et al.* (2014)	3D full plant topology	Peach	Carbon	–	–
AmapSim	Barczi *et al.* (2008)	3D shoot or root	Generic	Water or carbon (by coupling)	–	–
Piaf-Munch[b]	Lacointe and Minchin (2008)	3D full plant topology	Small plants	Water and carbon	Upon request	GUI, Command Line
–[b]	Janott *et al.* (2011)	3D full plant topology	Generic	Water	Upon request	–
This work[a]		3D full plant	Generic	Water and carbon (by coupling)	Open source	GUI, iPython notebook, Web interface

[a]Models with both 3D topology and 3D geometry.

[b]Models simulate interactions between carbon and water.

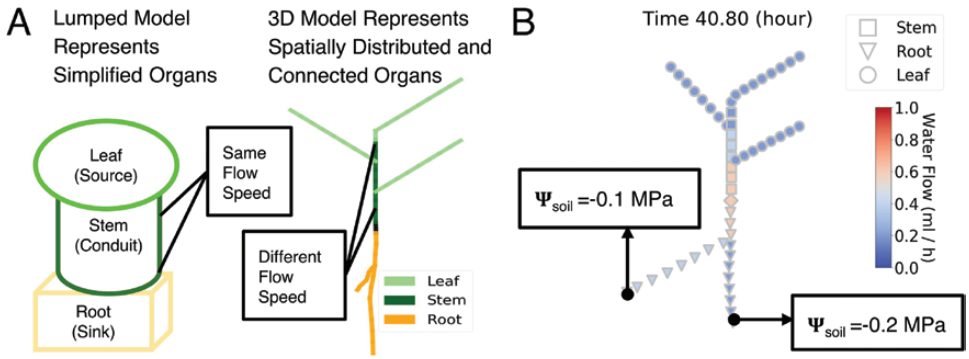

Figure 2. (A) The flow rate in lumped model depends only on the radius of the segment. In 3D models, branching structures affect flows as well. (B) On 3D structures, the heterogeneous soil water potential affects xylem water flows. Root in wet soil has more water flow compared to root in dry soil.

Here, we introduce a new functional-structural whole-plant modelling framework — CPlantBox. The novelty of CPlantBox is 2-fold. Firstly, CPlantBox can simulate the full plant structure at vegetative growth as a single topological network of organs (both root and shoot). The simulated plant architecture is composed of nodes or coordinates, then the nodes' properties and interactions scaled up to form the network. Secondly, CPlantBox provides a framework to couple with external models. In this paper, the framework provides the interface with the carbon and water flow model, PiafMunch (Website 1, PiafMunch is available upon request by contacting co-author A.L.) (Lacointe and Minchin 2008; Minchin and Lacointe 2017). The coupling of CPlantBox and PiafMunch (called CPlantBox–PiafMunch in the later text) enables fast simulations on large or complex plant structures, which was difficult to achieve before (PiafMunch uses manually defined plant architecture). Previously, PiafMunch was already able to simulate simple 3D plant topology. Now, by coupling with CPlantBox, an additional 3D geometry layer is added to PiafMunch. Here, we demonstrate the capabilities of the coupled model to generate a variety of plant structures and to reproduce realistic water and carbon flow behaviours.

MATERIALS AND METHODS

Description of CPlantBox

CPlantBox is an extension of the model CRootBox (Schnepf *et al.* 2018). CRootBox is a fast and flexible FSPM focusing on root architecture and root–soil interaction. We took advantage of the object-oriented structure of CRootBox to add new modules to represent the different shoot organs (Fig. 3B). The main extensions in CPlantBox are:

- CPlantBox can simulate realistic plant shoots and roots as a single-connected network. The output can be coupled with water and carbon flow simulations (Fig. 3C and D).
- As we move from root simulation to a full plant simulation (Fig. 3B), more complex relationships between the different organs have been included in the model. For instance, roots can now grow from seed, roots or shoot organs (Fig. 3B).
- The input parameter files are now XML-based (Fig. 3A). Comparing to plain-text parameters, XML increases the robustness, flexibility (more parameters for the shoot) and readability. Backward compatibility with previous parameter file (from CRootBox) was insured.

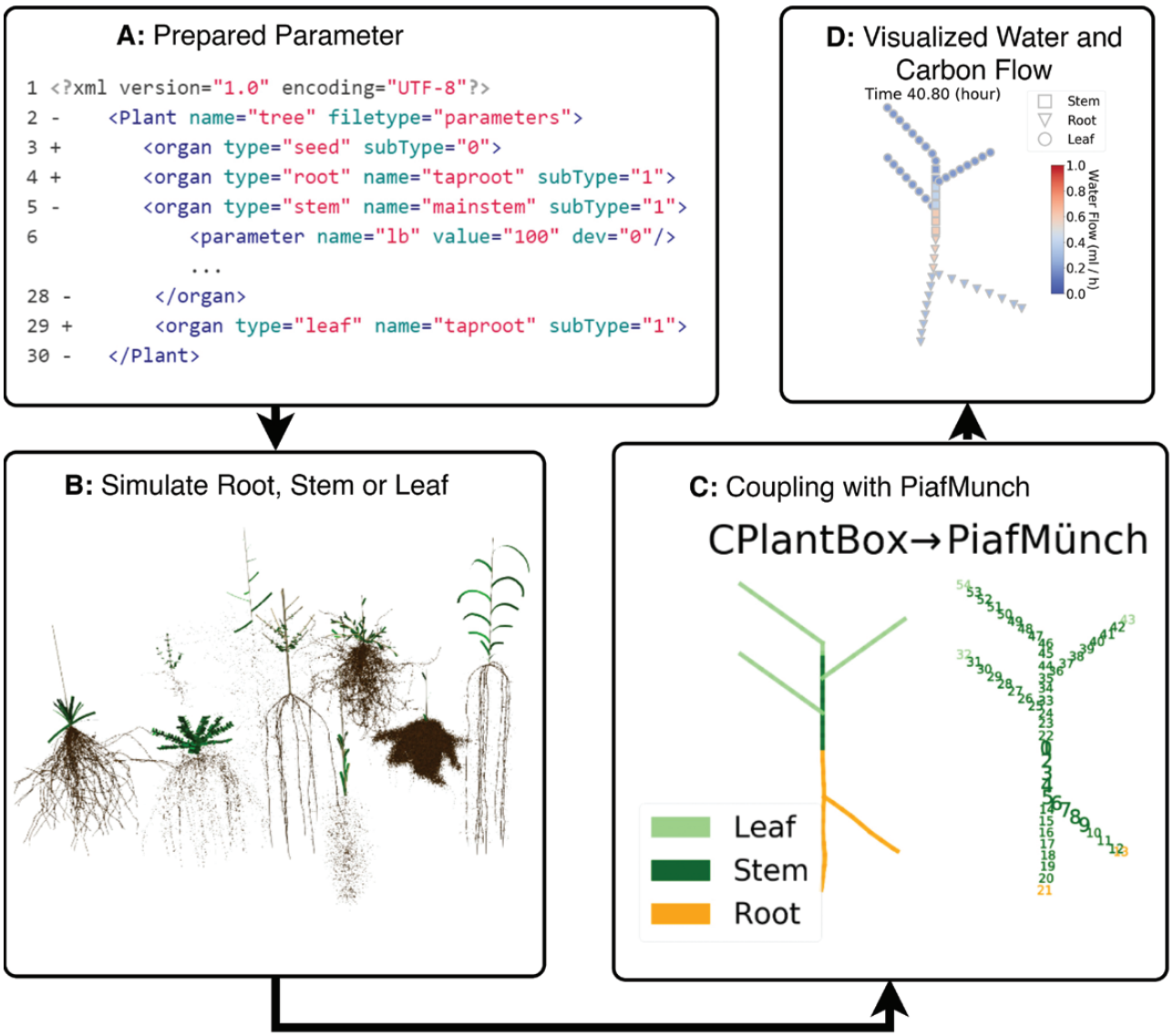

Figure 3. Flow chart of four major steps in CPlantBox–PiafMunch coupling. (A) Input parameter example (organ parameters with '+' sign means it is collapsed). (B) Output of CPlantBox is visualized. (C) Coupling between CPlantBox and PiafMunch, where output of CPlantBox can be the input file of PiafMunch. (D) Water flow output example from the CPlantBox–PiafMunch coupling.

The output of CPlantBox is a 1-dimensional network (with 3D geometry coordinates) (Fig. 3C). Each node of the network has 3D (3-dimensional) coordinates and other properties, such as an *organtype* (which indicates if it belongs to root, stem or leaf), a radius (or width) and a water potential, etc. The output format of the structure includes RSML (Lobet *et al.* 2015), VTP (Ahrens *et al.* 2005) and PiafMunch input format. After the plant structure is simulated (Fig. 3B, potentially thousands of segments), an input file for the PiafMunch can be generated. Afterwards, PiafMunch can be called by CPlantBox to read the input file, run simulations and generate the output files. At the end of the simulation, output files can be interpreted and visualized either internally or externally.

The current coupling is done by file-exchange and command-line-automation. Simulating the carbon and water flow within a 300-segments plant for 100 h growth time takes around 1 min (dependent on parameter setting) on a regular laptop (CPU: Intel Core i5-6300U 2.4 GHz, RAM 8 GB 2400 MHz). We also created functions to run simulations in batch processes. Installation, pre-processing, post-processing and visualization are exemplified in a Jupyter notebook (Website 2).

Description of PiafMunch

In PiafMunch (Lacointe and Minchin 2008; Minchin and Lacointe 2017), cohesion–tension theory is a precondition of the Münch

theory. The cohesion–tension theory states that xylem water flow is driven by water potential differences in the xylem. The water potential in general can be defined as the sum of partial water potentials: the gravimetric water potential: Ψ_z (MPa), the pressure water potential: Ψ_p (MPa) and the osmotic water potential: Ψ_o (MPa). According to the cohesion–tension theory, the pressure in the water can be smaller than zero such that a tension instead of a pressure is applied to a water body. It must be noted that the water pressure is expressed as the difference between the water pressure and the atmospheric air pressure. Following this definition, a positive pressure corresponds with a pressure in the water that is larger than the atmospheric pressure and a negative pressure with pressure that is smaller than the atmospheric air pressure. If dissolved substances flow freely within the xylem and phloem tissues, a gradient in concentrations or corresponding osmotic water potentials will not drive a flow within these tissues. Thus, the volume flow between two connected xylem's nth and $(n+1)$th segments ($J_{w\_xyl,n,n+1}$ mL h^{-1}) can be written as:

$$J_{w\_xyl,n,n+1} = \frac{\Delta P_{xyl,n,n+1}}{r_{xyl,n,n+1}} \tag{1}$$

where $r_{xyl,n,n+1}$ (MPa h mL^{-1}) is the xylem resistance and $\Delta P_{xyl,n,n+1} = (\Psi_{z\_xyl,n} + \Psi_{p\_xyl,n}) - (\Psi_{z\_xyl,n+1} + \Psi_{p\_xyl,n+1})$, $\Delta P_{xyl,n,n+1}$ is the difference between the sum of pressure and gravimetric potentials at the $(n+1)$th and nth segments, respectively. Similarly, the volume flow between two connected phloem sieve tubes $J_{w\_st,n,n+1}$ is:

$$J_{w\_st,n,n+1} = \frac{\Delta P_{st,n,n+1}}{r_{st,n,n+1}} \tag{2}$$

where $r_{st\_n,n+1}$ (MPa h mL^{-1}) is the total sieve tube (include sieve plate) resistance between nth and $(n+1)$th segment and $\Delta P_{st\_n,n+1} = (\Psi_{z\_st,n} + \Psi_{p\_st,n}) - (\Psi_{z\_st,n+1} + \Psi_{p\_st,n+1})$, $\Delta P_{st\_n,n+1}$ is the total potential difference between the neighbouring sieve tube segments, nth and $(n+1)$th. At the nth segment, the volume flow between the neighbouring xylem and phloem, which are separated by a semipermeable membrane, $J_{w\_lat,n}$ can be written as:

$$J_{w\_lat,n} = \frac{(\Psi_{p\_xyl,n} + \Psi_{o\_xyl,n}) - (\Psi_{p\_st,n} + \Psi_{o\_st,n})}{r_{lat,n}} \tag{3}$$

where $\Psi_{p\_xyl,n}$ is the water pressure potential in xylem and $\Psi_{p\_st,n}$ is the water pressure potential in sieve tubes, $\Psi_{o\_xyl,n}$ is the osmotic water potential in xylem and $\Psi_{p\_st,n}$ is the osmotic water potential in sieve tubes, $r_{lat,n}$ is the resistance of the membrane between xylem and phloem. Here, we should notice that, at the source location, osmotic pressure drives the $J_{w\_lat,n}$. But, at the sink location, the driving force is mainly the pressure water potential, because most osmotic water potential is removed by the unloading of carbon.

The water mass balance of xylem is:

$$\Delta J_{w\_xyl,n} + J_{w\_lat,n} = 0 \tag{4}$$

where $\Delta J_{w\_xyl,n}$ is the xylem water flux divergence, either depletion or accumulation, over segment n. $J_{w\_lat,n}$ is the xylem water flux exchange between phloem. The xylem water divergence can be written as $\Delta J_{w\_xyl,n} = J_{w\_xyl,n,n+1} - J_{w\_xyl,n-1,n}$. The depletion of xylem water occurs at the source, often the leaves, where water transpired into the atmosphere or goes to phloem ($J_{w\_lat,n}$). The accumulation occurs at the sink, often the roots, where water comes from the soil or the phloem ($J_{w\_lat,n}$). Similarly, the water mass balance of phloem can be written as:

$$\Delta J_{w\_st,n} - J_{w\_lat,n} - NZS_n = 0 \tag{5}$$

where $\Delta J_{w\_st,n} = J_{w\_st,n,n+1} - J_{w\_st,n-1,n}$ is the flux divergence, either depletion or accumulation, over phloem sieve tube. The depletion of phloem sap occurs at the sink, where carbon is unloaded from the phloem and water goes back to xylem. The accumulation occurs at the source, where water goes from xylem to phloem and carbon is loaded to the phloem. NZS_n is the non-zero sugar volume flow accompanying $J_{s\_lat,n}$. At the source location, $NZS_n = \bar{V} \cdot J_{s\_loading,n}$, $\bar{V}$ is the non-zero partial molar volume of sucrose, $J_{s\_loading,n}$ (mmol h^{-1}) is the loading rate from the source tissue (e.g. parenchyma) to the phloem at the nth node. At the sink location, $NZS_n = -\bar{V} \cdot J_{s\_loading,n}$, $J_{s\_unloading,n}$ (mmol h^{-1}) is the loading rate from the phloem to the sink tissue.

The mass balance of sucrose can be written as:

$$J_{s\_(un)loading} + J_{w\_st,n-1,n} \cdot C_{st,n-1} - J_{w\_st,n,n+1} \cdot C_{st,n} = 0 \tag{6}$$

where $J_{s\_(un)loading}$ is the source (sink) term. It could be zero at transportation segments, or positive value at source or negative value at sink. $C_{st,n-1}$ is the sucrose concentration at the $(n-1)$th node, the concentration multiplied by $J_{w\_st,n-1,n}$, which is the phloem (or sieve tube) flow from $(n-1)$th node to the nth node, will give us the carbon mass increase from $(n-1)$th node to the nth node. The $C_{st,n}$, which is the sucrose concentration in the nth node, multiplied by $J_{w\_st,n,n+1}$, which is the phloem (sieve tube) solute flow from nth segment to the $(n+1)$th segment, will give us the carbon mass loss from nth segment to the $(n+1)$th segment.

Comparison with experimental results

Recently, Knoblauch *et al.* experimentally tested the Münch theory on morning glory (*Ipomoea nil*) (Knoblauch *et al.* 2016). To validate the functions of CPlantBox–PiafMunch and estimate carbon loading/unloading speed, we decided to perform a re-analysis of their experimental data set (measurements are shown in Table 2). In particular, we used one set of morning glory experimental data (left column of 7.5 m morning glory in Table 2) for calibration and another set (right column of 7.5 m morning glory in Table 2) for validation of our modelling system. We choose to use these data sets for different reasons. Firstly, the experimental measurements match almost directly both the input and output of the CPlantBox–PiafMunch model (Fig. 4). Secondly, the authors performed a variety of experimental treatments, allowing us to parameterize our model on one experiment and validate on the others. Finally, the relatively simple architecture of the morning glory allowed us to focus our analysis on the resolution of carbon and water flow themselves, not the architecture.

Table 2. List of experimental measurements done by Knoblauch *et al.* (2016), other parameters used for simulation are summarized in Table 3.

Measurements	Measurements on 7.5 m morning glory	Measurements on defoliated morning glory
Architecture	Idealized schematic drawing (Fig. 10A)	Idealized schematic drawing (Fig. 10B)
Sieve-tube conductivity (k_{st})	At 1, 4 and 7 m location	When plant is 18 m long
Pressure (P)	Leaf phloem turgor pressure is measured at 1st, 3rd, 5th, 9th and 10th leaf (blue dots in Fig. 10C). Root turgor pressure is measured in the cortex of elongation zone.	Leaf phloem turgor pressure is measured at bottom leaf of the 4 m foliated stem when plant is 2.5, 3.5, 9, 10 and 14 m long (blue dots in Fig. 10D)
Phloem sieve-tube flow speed (U_{st})	Between second and third leaf (arrows in Fig. 10C)	When plant is 18 m long
Viscosity (η)	Assume constant at 1.7 mPa·s	Assume constant at 1.7 mPa·s

In a first experiment (that we used for the parameterization of our simulations is shown in Table 2 and illustrated in Fig. 10A), the authors measured the permeability of sieve tubes at three locations (1, 4 and 7 m) on a 7.5 m tall morning glory (referred to as 7.5 m plant in following text). The phloem pressure and phloem flow rates were also measured in the same plant.

In a second experiment (that we used for validation shown in Table 2 and illustrated in Fig. 10B), another morning glory plant was continuously defoliated except for the top 4 m (this plant is referred to as *defoliated plant*). When the defoliated stem was 2.5, 3.5, 9, 10 and 14 m long during its growth, the pressure of the bottom leaf was measured.

Details about the exact data transformations performed between the experimental measurements and the model parameters can be found in the **Supporting Information File S1**.

RESULTS

In the following section, five functions of CPlantBox are exemplified and the results created by those functions are showcased. Structurally, a wide variety of whole-plant architectures are simulated by CPlantBox in example 1. Functionally, we evaluated water and carbon simulations of a three-leaf-two-root plant under either homogeneous or heterogeneous environments in examples 2 and 3. Quantitative comparisons between simulations and experimental data are shown in examples 4 and 5.

Example 1: simulation of contrasted plant architectures with CPlantBox

Plants display a variety of forms and architectures, both above- and below-ground (Barthélémy and Caraglio 2007). Stem branching patterns are important factors determining the above-ground architecture of plants. Figure 5A shows an example of three branching patterns generated by CPlantBox using different parameter files. A second important determinant of the above-ground architecture is the arrangement of the leaves on the stems. Figure 5B includes three leaf arrangements created by only changing single input parameter. By combining different branching patterns and leaf arrangements, we extended existing CRootBox outputs (Schnepf *et al.* 2018) into full plant architectures (Fig. 6). It is worth mentioning here that each unique structure is obtained solely by changing the input parameter files. The source code itself is not modified. This level of flexibility is more friendly to the end-users.

Example 2: simulation of water and carbon flow with the coupled model CPlantBox–PiafMunch

We created a small plant (three leaves and two roots) to simulate carbon and water flow (Fig. 3C and D). The input and output parameter values were collected from various sources from the literature (summarized in Table 3) (Zwieniecki *et al.* 2001). The simulated values of xylem pressure, flow rate and hydraulic conductivities are within the range of literature values. For example, xylem can sustain flow under pressure between −2.0 and −8.0 MPa, before losing 50 % of its conductivity (Martínez-Vilalta *et al.* 2002). The simulated xylem water flow rate is typically around 1 mL h^{-1}.

The transpiration rate on each leaf was set to mimic diurnal flow patterns. We set the transpiration rate to 0.2 mmol h^{-1} (0.0036 mL h^{-1}) per leaf during daytime (from 0500 to 1730), and to 0 at night-time (from 1730 to 0500 the next day). As shown in Fig. 7A, pressure is decreasing from root to leaf. Xylem flow during the day is caused by transpiration, and the water flow going back into the xylem caused the xylem flow at night (which are lower than 0.0005 mL h^{-1}, can be visible when zoom in Fig. 7B). There are water moving from xylem to phloem at the source. Indeed, as the carbon is loaded into the phloem, it reduces the sieve tube water potential. The water crosses the membrane and moves from xylem to phloem. Therefore, we can observe that phloem carbon flow rates are affected by the diurnal xylem water flow (Fig. 7D).

The loading rate into the phloem at source location is set to a constant value during both day and night. This is consistent with experimental data (Stitt *et al.* 2010; Streb and Zeeman 2012; Pokhilko and Ebenhöh 2015), as starch is degraded at night and the generated sucrose can be loaded into the phloem to sustain the flow.

Example 3: simulations of water and carbon flows in response to heterogeneous environments

Heterogeneous environments can have a large impact on plant growth and development. 4D FSPM can be used to simulate and visualize such environmental impact. To observe the effect of heterogeneous soil water availability on the carbon flow within the root system, we manually assigned two different soil water potentials at two root tips

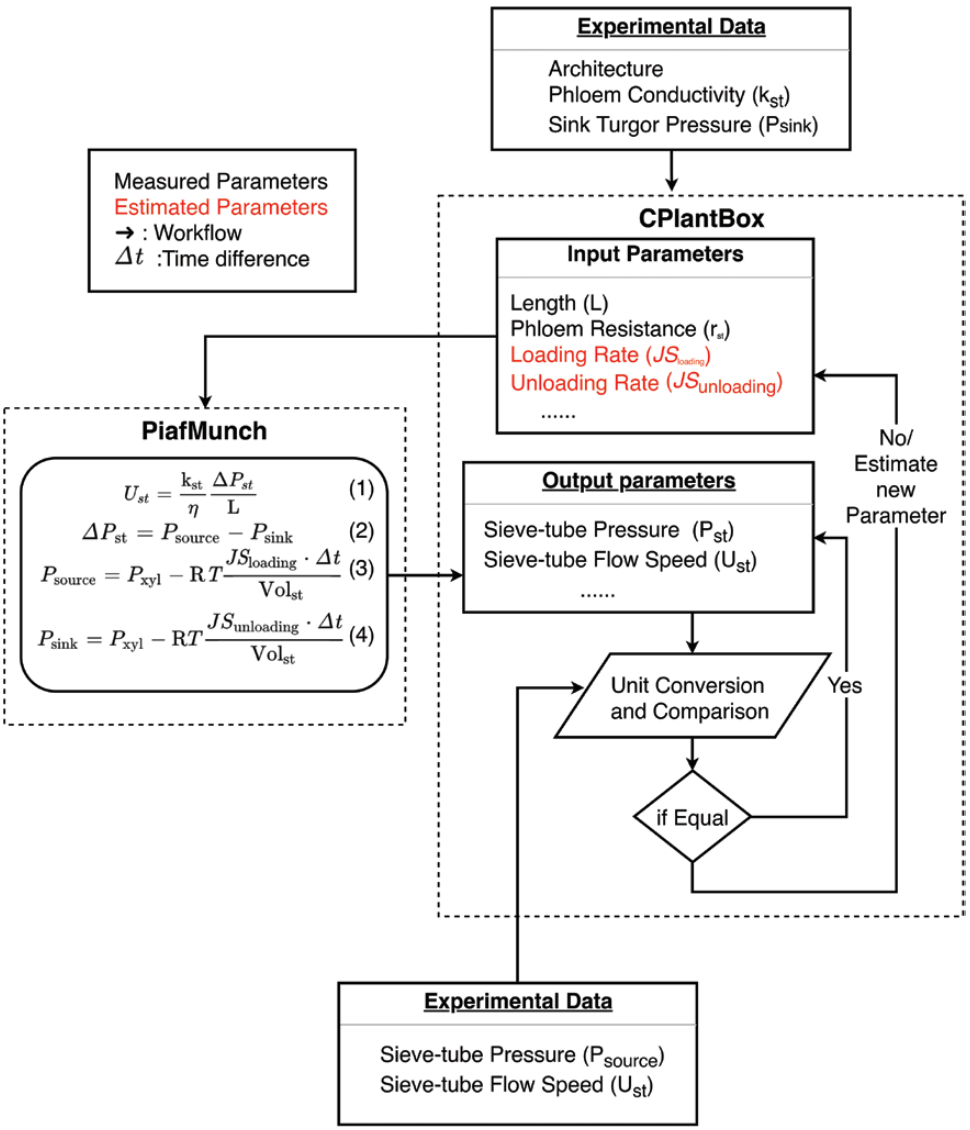

Figure 4. Measured parameters (in black text) and estimated parameter (in red text) in comparison with experiment. Length is calculated from simulated architecture (left side of Fig. 10A and B), which is based on the schematic drawing (right side of Fig. 10A and B). r_{st} is converted from measured k_{st} [see Supporting Information—Equation 7]. Pressure difference (ΔP_{st}) is the phloem source pressure (P_{source}) minus phloem sink pressure (P_{sink}). R is the universal gas constant and T is the absolute temperature. P_{xyl} is the pressure of xylem at source or sink location, those pressures are calculated by carbon loading rate ($J_{s\_loading}$) and carbon unloading rate ($J_{s\_unloading}$). Arrows highlight our modelling workflow. ΔT is the time difference, Vol_{st} is the sieve tube volume. Units are in Table 3 and Supporting Information. The fitting of loading and unloading rate to source phloem pressure and flow rate is shown at the end of Supporting Information File S1.

(bottom root in blue colour with −0.2 MPa, upper root in red colour with −0.4 MPa in Fig. 8A). In Fig. 8B, we observe a pressure difference between two roots, which causes hydraulic redistribution at night from the wet to the dry parts of the root system (Fig. 8C). During the day, the water flow to the wet part is larger than the flow to the root in the dry soil. We also observed that the carbon concentration in the high water potential root is lower (red line in Fig. 8D). In Fig. 8F, we can see that total carbon flow in wet root is lower than the flow in the dry root.

Different temperature or developmental stages can also cause heterogeneous leaf transpiration rate. We assigned the 0.3 mmol h^{-1} (0.0054 mL h^{-1}) transpiration on the top left leaf (higher transpiration leaf in Fig. 9A with red colour), 0.2 mmol h^{-1} (0.0036 mL h^{-1}) transpiration on the right leaf (middle transpiration leaf in Fig. 9A with green colour), 0.1 mmol h^{-1} (0.0018 mL h^{-1}) transpiration on the bottom left leaf (lower transpiration leaf in Fig. 9A with blue colour). In Fig. 9B and C, we can observe the pressure and flow gradient of three leaves at

Table 3. Literature values and simulation parameter values used for small plant, 7.5 m plant and *defoliated plant*.

Parameter	Symbol	Type	Experimental range	Unit	Small plant	7.5 m plant	Defoliated plant
Xylem[a] resistance	r_{xyl}	Input	0.011 to 3.3 by stem (Sellin 1993)	MPa h mL^{-1}	2.08 by stem 6.9 × 10^{-2} by segment (0.25 cm)	0.081 by stem 0.0005 by segment (5 cm)	0.071 to 0.191 by stem 0.0005 by segment (5 cm)
Phloem[b] resistance	r_{phl}	Input	40 to 90 (Knoblauch *et al.* 2016)	MPa h mL^{-1}	70 by segment (0.25 cm)	Fig. S1 in Supporting Information	Fig. S1 in Supporting Information
Transpiration[a]	–	Input	0 to 1 × 10^{6} m^{-2} (Wullschleger *et al.* 2000; Almeida *et al.* 2007)	mmol h^{-1}	0.2 or diurnal	0.2	0.2
Soil water[b] potential	–	Input	−0.2 to −0.8 (Draye *et al.* 2010; Lobet *et al.* 2014a)	MPa	−0.6	−0.6	−0.6
Loading rate[c]	$J_{s\_loading}$	Input	–	mmol h^{-1}	0.0007 on each source segment	6.4 × 10^{-6} on each source segment	6.4 × 10^{-6} on each source segment
Unloading[c] rate	$J_{s\_unloading}$	Input	–	mmol h^{-1}	0.00028 × C_{st}[d]	0.012 × C_{st}[d]	0.012 × C_{st}[d]
Xylem[a] pressure	P_{xyl}	Output	−0.2 to −8 (Martínez-Vilalta *et al.* 2002)	MPa	0 to −0.7	0 to −0.7	0 to −0.7
Phloem[b] pressure	P_{phl}	Output	0 to 1.44 (Savage *et al.* 2017)	MPa	0 to 1.8	0 to 1.4	0 to 1.8
Xylem water[a] flow rate	J_{w_xyl}	Output	0 to 3.6 (Zwieniecki *et al.* 2001)	mL h^{-1}	0.20 to 0.62	0 to 1.2	0 to 1.2
Phloem solut[b] flow rate	J_{w_st}	Output	−0.02 to 0.02 (Windt *et al.* 2006; Comtet *et al.* 2017)	mL h^{-1}	−0.001 to 0.0006	−0.002 to 0.0006	−0.002 to 0.0006
Phloem[b] carbon flow rate	J_{s_st}	Output	–	mmol h^{-1}	0 to 0.00022	0 to 0.00022	0 to 0.00022

[a]Estimated input parameters that falls into literature range.

[b]Parameters equal to Knoblauch's measurements.

[c]Calibrated parameters through Knoblauch's 7.5 m plant measurements, unchanged on defoliated plants.

[d]C_{st}: carbon contraction in sieve tubes (details in **Supporting Information**, Equation 11).

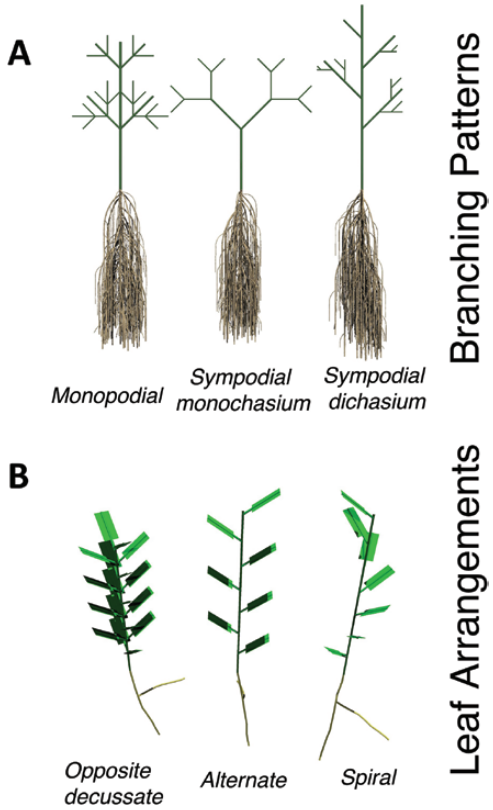

Figure 5. (A) Simulated stem branching pattern simulated by CPlantBox; (B) leaf arrangements simulated by CPlantBox.

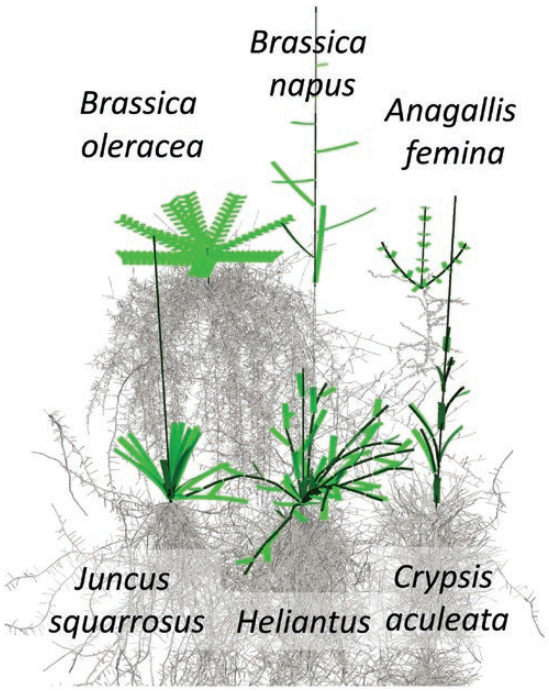

Figure 6. Simulated whole-plant structures. *Brassica oleracea*, *Brassica napus*, *Anagallis femina*, *Juncus squarrosus*, *Heliantus* and *Crypsis aculeate*.

different transpiration rate. In Fig. 9D and E, we observe that carbon concentrations are different, but total carbon flows are only slightly different between the different leaves as loading rate is kept constant. In Fig. 9F, we can see that, when transpiration changes between day and night, the carbon flow in high transpiration leaf is more sensitive to the changes. However, the total carbon flow did not change significantly. In this example, we kept the loading and unloading speed homogeneous and constant. It is because physiologically the starch degradation will compensate a temporal loss on the leaf level, just the same as the night carbon loading (Savage *et al.* 2016; Zhang *et al.* 2016). The carbon loading is likely to decrease in the long term, but it might not take effect in a few days.

Example 4: predicting carbon loading and unloading for contrasted morning glory shoot architectures in morning glory

To assess whether CPlantBox–PiafMunch was able to simulate realistic carbon and water flow values, we simulated experiments conducted with morning glory (Knoblauch *et al.* 2016). In order to simulate Knoblauch *et al.*'s experimental results on the morning glory, six virtual plants with contrasted architectures were created (Fig. 10). The architecture's parameterization is based on the idealized schematic of the original paper. As described in Table 2, the reference plant was 7.5 m long, with 12 homogeneously distributed leaves and one shoot tip (Fig. 10A). The *defoliated plants* each had four leaves and one shoot tip near the apex of the stem, with different length for the defoliated section (Fig. 10B).

Regarding the physiological parameterization for the carbon and water flow simulation, in both the experiments and the modelling exercise, the morning glory was simplified to 1-source-1-sink system. Therefore, we assumed that the 12 leaves and the shoot tip are all homogeneous sources with the same carbon loading rate. The carbon unloading rates in the sinks were also considered homogeneous. Thus, we could create a 1-source-1-sink scenario as shown in Fig. 10C, where all leaves together are counted as one source and all the roots together count as one sink.

As shown in Figs 10C and 4, we used the measured pressure and measured flow rate to find our initial input parameters, in particular the carbon loading and unloading rate. We estimated the corresponding loading and unloading rate using a least square fitting (lower part of Fig. 10C, details are in Supporting Information—Table **S**1).

The carbon loading and unloading rate estimated on the 7.5 m plant was then applied on the *defoliated plants* (Table 2; Fig. 10D). None of the parameters used in 7.5 m plant simulations were modified except the plant structure (Fig. 10B). As shown in Fig. 10D, we could see that the simulated pressure values in the sieve tubes were in good agreement with the experimental values.

Example 5: studying source–sink relations at the organ level in morning glory

In the previous section, the plant architecture was simplified to a 1-source-1-sink structure (Fig. 10C), as same as the experimental data

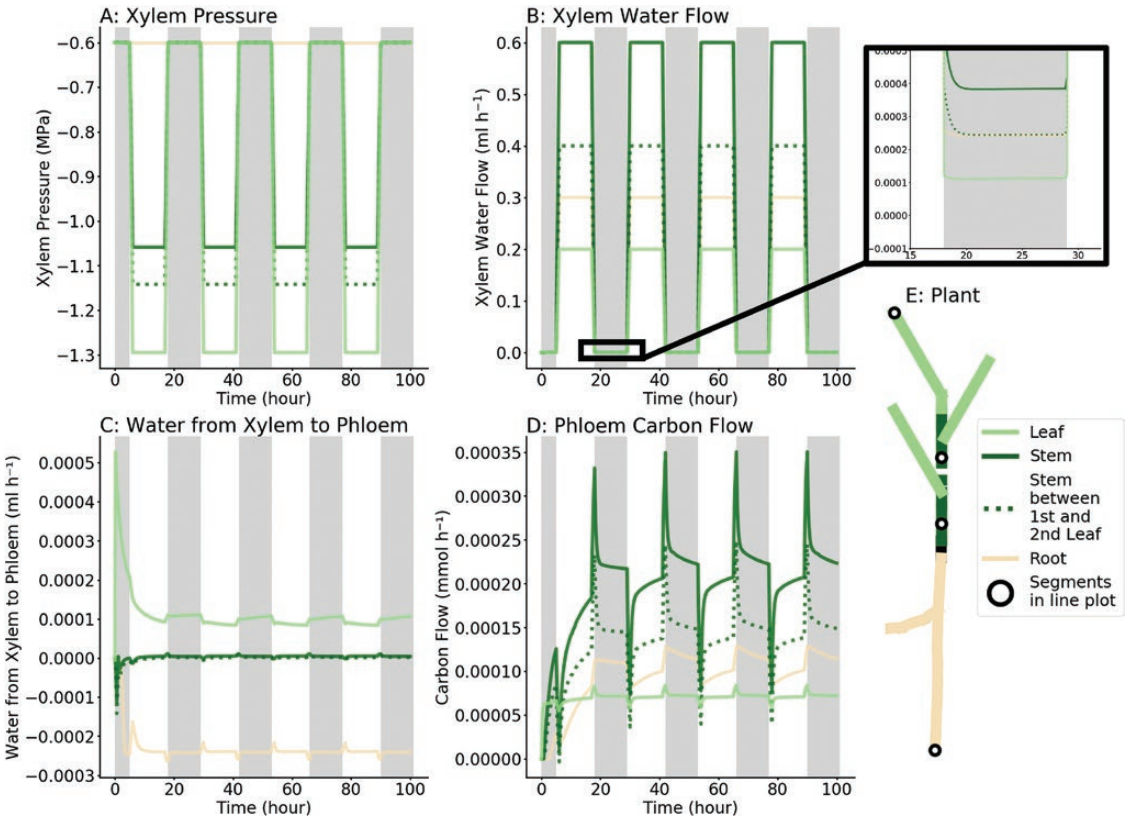

Figure 7. (A) Transpiration creates xylem pressure gradients during the day, whereas the pressure remains comparatively stable during the night. (B) The pressure gradient caused xylem water flow during daytime, the water flow at night is low, it is the water flow from phloem to xylem. (C) The water flows from xylem to phloem at source location, whereas it flows from phloem to xylem at sink location. (D) Phloem (sieve tube) carbon flow fluctuations are caused by diurnal xylem water flow, the trend of changing is qualitatively consistent with previous studies (Stitt *et al.* 2010; Streb and Zeeman 2012; Pokhilko and Ebenhöh 2015). (E) Plant structure where the colours correspond to the flow figures from (A) to (D), the dashed line shows the segments between the first and second bottom leaves. The flows going to circled segments are also shown as dashed lines in (B) and (D). The pressure or flow exchanges of the circled segments are shown in (A) and (C). The loading rate inside the phloem at source location is set to constant during both day and night, because starch is degraded to sucrose and then loaded into the phloem at night (Stitt *et al.* 2010; Streb and Zeeman 2012; Pokhilko and Ebenhöh 2015).

analysis (Knoblauch *et al.* 2016). We wondered if the model would be able to simulate the detailed relationship between different leaves inside the single source. It should be noticed that, as the large variance between the leaves might be caused by experimental variations, such detailed fitting might not be biologically relevant. However, it remains an interesting conceptual exercise, to test the flexibility and capabilities of our models.

We reused the calibration obtained on the 7.5 m plant (Fig. 10A and C). As shown in Fig. 11A, it is obvious that the simulated pressure in each single leaf does not fit the measured pressure. Therefore, we fitted each single leaf pressure by assigning independent carbon loading and unloading rate. We observed that, when we reached a good fit on Fig. 11B, the directions of individual flows changed significantly compared to the flow when fitting the parameters globally (lower line plot of Fig. 10C). Indeed, with the individual fitting, some leaves become carbon sinks instead of being carbon sources. In Fig. 11D, the red arrows indicate a change on the carbon flow directions compared to the 1-source-1-sink scenario, as well changes in the total carbon loading (Fig. 11C).

DISCUSSION

CPlantBox generates full plant architectures

Historically, root and shoot models have been developed independently. Most models indeed focus on either part of the plant, representing the other one as a boundary condition. Some existing models are able to simulate both root and shoot, but for specific plant species (Drouet and Pagès 2003; Lacointe and Minchin 2008; Janott *et al.* 2011; Da Silva *et al.* 2014; Lobet *et al.* 2014b). Here, we presented CPlantBox, the first model, to our knowledge, able to represent both root and shoot, as a single network, for a variety of plant species (see example 1 in the Results section, and Figs 5 and 6).

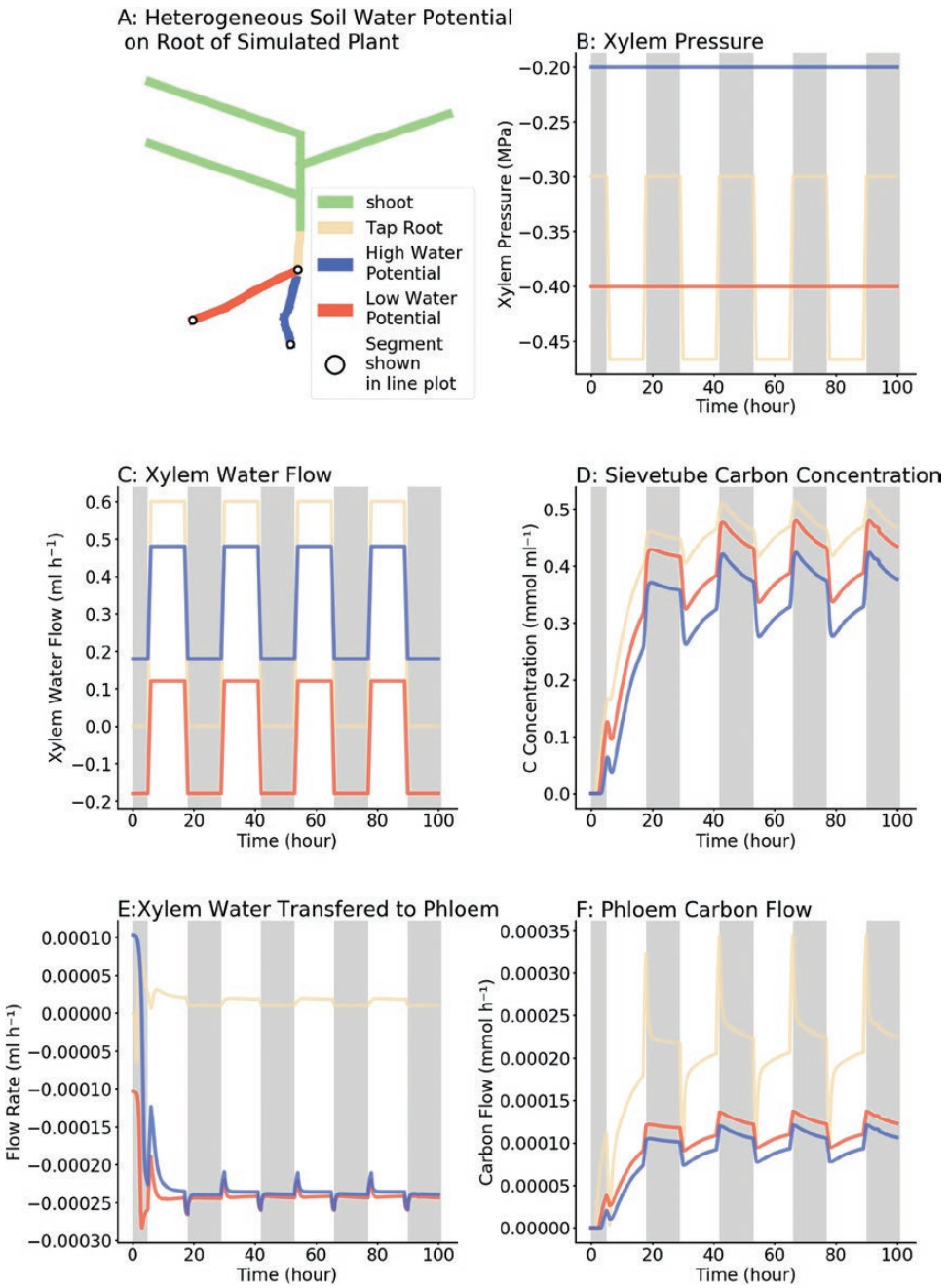

Figure 8. (A) Soil water potential around the lower root (blue colour) is higher than the upper root (red colour). (B) Pressure values at the boundary location are different according to the higher or lower soil water potential. (C) The bottom root (blue colour, in wet soil) xylem has higher water flow. The flow rate in upper root (red colour) is negative at night. It means that, at night the water is coming out from the upper root to the soil, which is also called the hydraulic redistribution (in other words, the plant root system behaves as a pathway for water flow from wet to dry (or salty) soil areas). (D) Carbon concentration in the dry (upper) root is higher than the wet root. (E) Water flows from xylem to phloem at sink location only in the wet root (blue line) shortly at the beginning, then water flows from phloem to xylem in both roots at a similar rate. (F) Carbon flow decreased in the high water potential (lower) root phloem.

CPlantBox was designed to be flexible and amenable for multiple plant studies. For the root part, CPlantBox inherited the flexibility of the model it was built upon, CRootBox. As CRootBox is able to generate any type of root architecture, so is CPlantBox. For the shoot part, we implemented several branching and leaf arrangement patterns. By combining these patterns, many types of shoot architectures can be simulated. Both root and shoot architectural parameters are defined into the model parameter file, making it easy to set-up and reproduce.

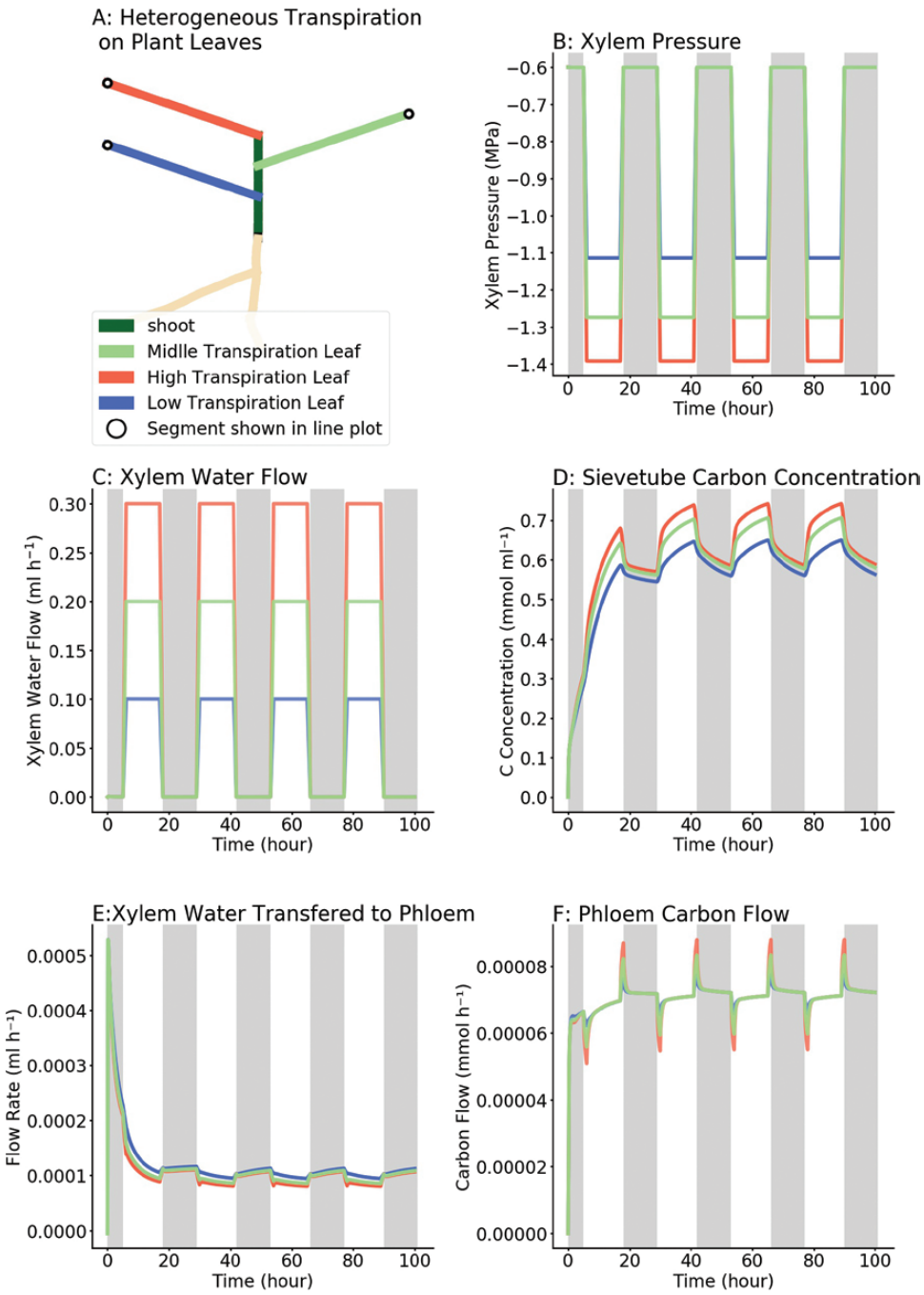

Figure 9. (A) The lower left leaf (in blue) has lower transpiration rate and the top left leaf (in red) has higher transpiration rate. (B) The pressure in each leaf is changed according to their transpiration rate. (C) The water flow in each leaf is changed according to the transpiration rate. (D) Carbon concentration on the higher transpiration leaf (red line) is higher. (E) Water going from xylem to phloem at source location is lower at the higher transpiration leaf (red line). (F) Carbon flow rates are the same at steady status, leaves with higher water transpiration (red line) are more sensitive to the changes.

CPlantBox–PiafMunch simulates water and carbon flow in the full plant

We combined CPlantBox with a mechanistic model of carbon and water flow: PiafMunch (Lacointe and Minchin 2008). The coupled model allowed us to simulate water and carbon flow within complex full plant architectures, which was not possible previously. In the Results section, we demonstrated four examples. Example 1 is focusing on structures, while example 2 focuses on diurnal carbon/water flow compared to literature measurements. Example 3 shows that the combinations of structures and functions could reproduce qualitatively

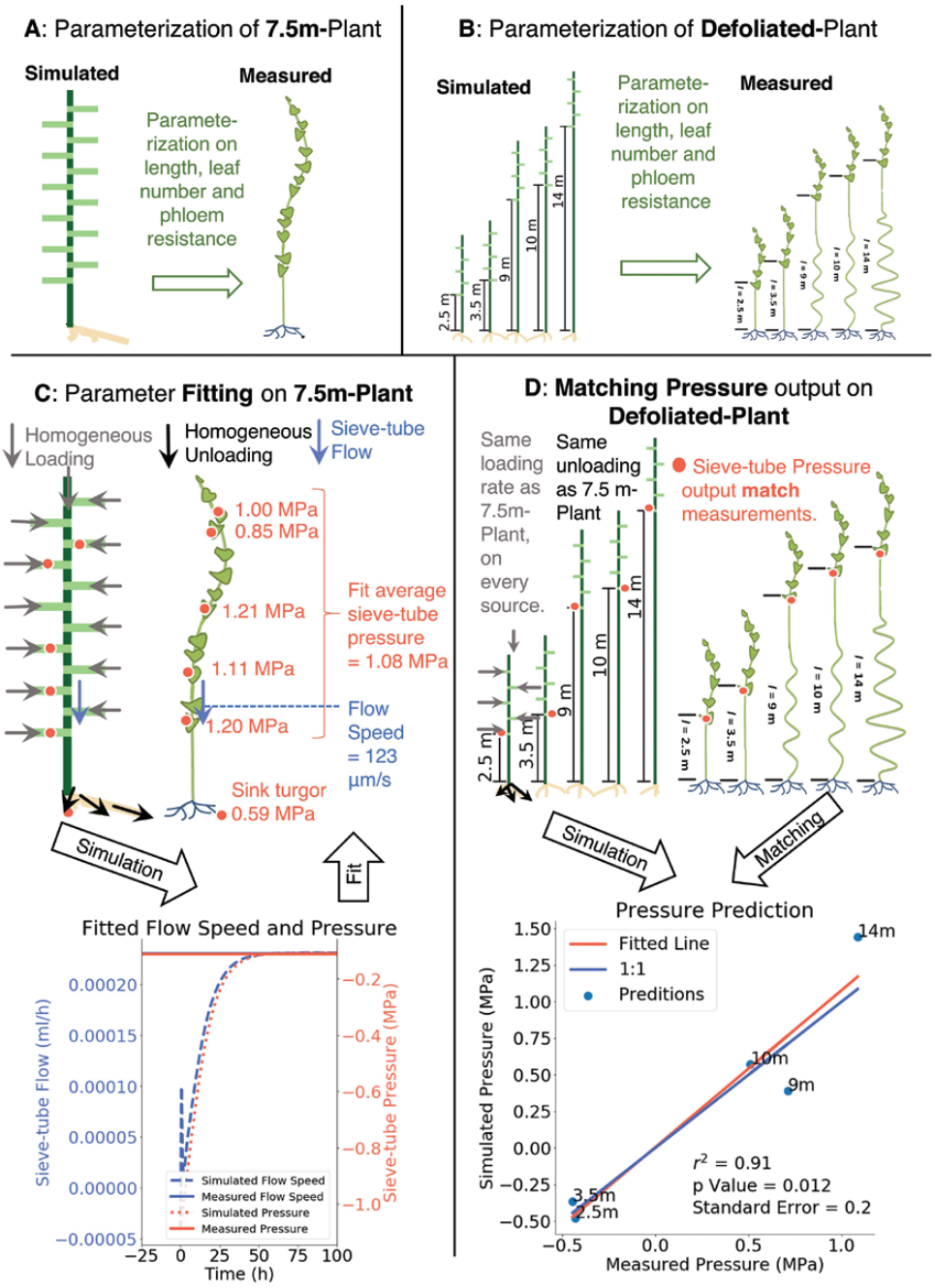

Figure 10. Steps of comparison between simulations and experiments. (A) One *in silico* plant structure (left) is created based on schematic drawing of the *7.5 m plant* (also shown in Supporting Information—Fig. S2). The resistance parameterization can be found on Supporting Information—Fig. S1. (B) Five *in silico* plant structures are created based on schematic drawing of *defoliated plant*. (C) In phloem, physiological parameters such as source average pressure (red) and sieve tube flow rate (blue) are fitted by applying homogeneous loading rate on each leaf, and homogeneous unloading rate at each root tip. Parameters can be found in Table 2, fitting of loading and unloading speed can be found in Fig. 4 and Supporting Information—Table S1. (D) By applying the fitted unloading rate and loading rate from 7.5 m plant on five *in silico* defoliated plants, simulated pressure values match the measured values from Knoblauch *et al.* (2016).

experiments from the literature. Example 4 reproduces the experimental results quantitatively, then in example 5 we used conceptual experiments to prove that the heterogeneous leaf environments (in example 3) can explain the experimental results.

In our simulations, we could observe a strong interplay between xylem and phloem flows. The diurnal transpiration patterns (the high peak in fluxes in the morning and the sharp decline when the light was stopped followed by an increase in flux during night) (Fig. 7) are

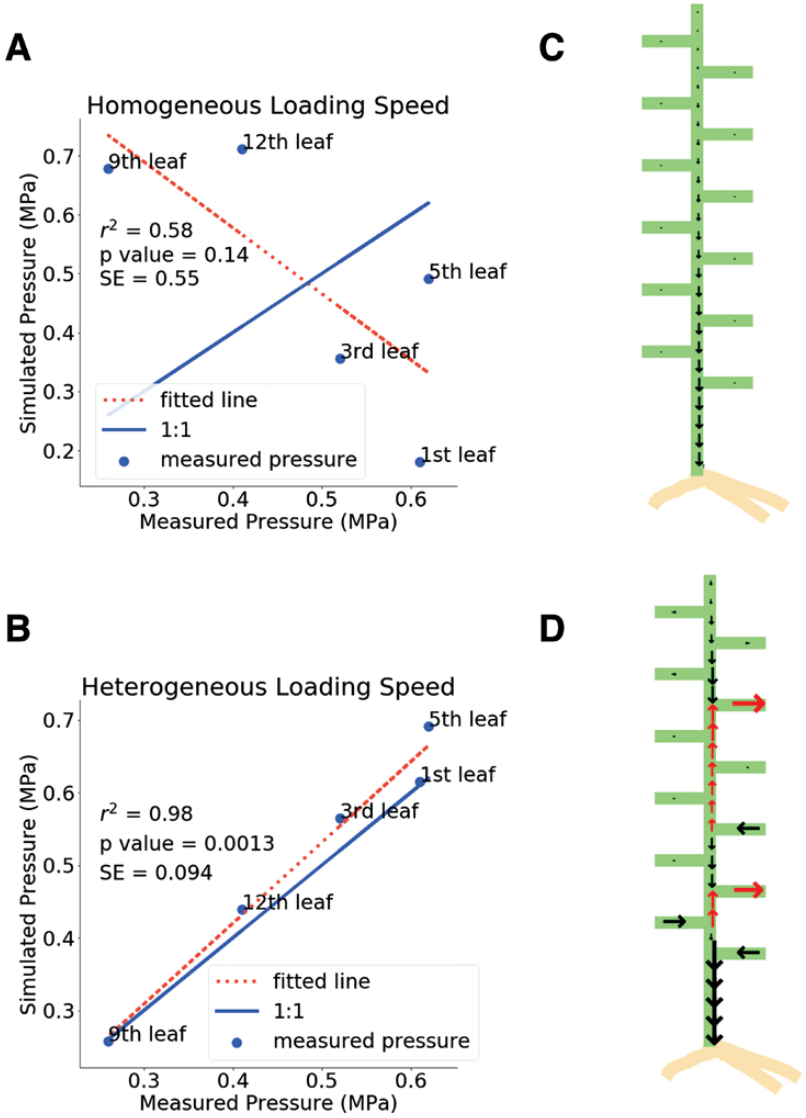

Figure 11. Comparison of simulations with (A) equal loading rate on all leaves to fit average pressure and (B) individual loading/unloading fitted pressure on each single leaf; (A) result for using homogeneous loading rate on each leaf; (B) fitted individual loading and unloading rate on each leaf; (C) flows are all heading to root when all leaves are sources with same loading rate (the scenario we used for parameter fitting); (D) flows directions changed (in red colour) when the individual leaf pressure is fitted (it is only one of the possible solutions, to show that we could change loading/unloading value on each source).

consistent with previous experiment and modelling (Pokhilko and Ebenhöh 2015). The low water potential in the xylem vessels during the day (as a result of the high transpiration rate) limits the water movement towards the phloem. During the night, as the stomata closes, the xylem water potential increases, leading to a higher water flow towards the phloem sieve tubes and a higher flow of carbon throughout the whole plant (Fig. 7D). However, the higher night carbon flow might also be caused by constant loading rate, whereas in some cases, the loading rate at night is reduced to 60 % of the day value (Kallarackal *et al.* 2012), so that the overall carbon flow may not be increased. In turn, the water flow from the xylem to the phloem induced a small upward water flow during the night, even in the absence of transpiration flux (Fig. 7B). These results from our coupled models are comparable to previous published modelling results (Lacointe and Minchin 2008, 2019; Minchin and Lacointe 2017) and are consistent with experimental data (see Table 2 for details) (Thorpe *et al.* 2011).

CPlantBox–PiafMunch considers the impact of heterogeneous environments

One of the main advantages of FSPMs is their ability to explicitly consider the influence of heterogeneous environments (in both space and time). In our third example, we used our coupled CPlantBox–PiafMunch modelling framework to simulate the influence of heterogeneous soil and atmospheric conditions on the carbon and water flows in the plant.

First, we imposed different soil water potentials to the different roots of our plant (Fig. 8A). In response to this heterogeneity, we could make two main observations. Firstly, root water potential and water flow (Fig. 8B and C) were directly influenced by the soil water potential. As the soil water potential decreases, the water flow in the xylem decreases. This is a well-known effect, observed both *in vivo* (Doussan *et al.* 2006; Garrigues *et al.* 2006) and *in silico* (Javaux *et al.* 2008; Meunier *et al.* 2016). Secondly, we observed that the carbon flow (Fig. 8F) in the phloem was inversely correlated with the soil water potential. Indeed, our simulation results show that carbon flow is slightly higher in the portion of the root system in contact with a dry soil (red line in Fig. 8F). This is due to the lower carbon concentration of root phloem in wet soil (blue line in Fig. 8D). The lower carbon concentration in wet root phloem (blue line in Fig. 8D) is a result of dilution by water from wet root xylem to wet root phloem along the root until the root tip (like tap root in light yellow colour). At the root tip, the unloading rate is proportional to the carbon concentration. Thus, the flow rates of two split root are similar. Because the flow rates are similar, but concentration is lower in the wet root, the total carbon flow is lower in the wet root (Fig. 8F). Again, this dynamic was observed experimentally for several plant species in split root experiment (William *et al.* 1991; Farrar and Jones 2000; Muller *et al.* 2011).

To simulate heterogeneous atmospheric environment, we imposed different transpiration rates to the different leaves of our plant (Fig. 9A). Like water potential change at the sink location, the transpiration rate at the source location directly induced changes of xylem pressure (Fig. 9B) and xylem water flow rate (Fig. 9C). Heterogeneous transpiration rates on leaves are also observed *in vivo* and simulated *in silico* (Sinoquet *et al.* 2001; Pincebourde *et al.* 2007). In Fig. 9D, we could observe that the carbon concentration in phloem is increased, because in Fig. 9E we could observe that in the high transpiration leaf (red line), less water is moving from xylem to phloem. This is because the water potential increases (red line in Fig. 9B) and pressure drops (red line in Fig. 9A) in the high water potential leaves. Thus, the final phloem carbon flow rate did not change at steady state (lines are aggregating in Fig. 9F).

Current limitations of the model and future perspectives

In this paper, we highlighted some of the capabilities of our new coupled model CPlantBox–PiafMunch. We have shown that we can simulate realistic water and carbon flow within a full plant structure. However, it is important to stress the current limitations and future developments of our model.

Firstly, all the simulations were done with static plants. At this stage, we did not explore the impact of the carbon distribution on the growth and development of the plant. The current version of CPlantBox platform simulates the flow of carbon based on predefined unloading parameters. In future modelling project, we are planning to compute the root carbon demand on a local (segment scale) basis. For instance, carbon transported to the root is also used for exudation and maintenance (Farrar and Jones 2000). In the future, we will explicitly connect the growth function in CPlantBox to the local carbon availability as prescribed by PiafMunch.

Secondly, in the presented simulations, the environment was static as well. In order to explore only the resolution of carbon and water within the plant, we did not connect our models to dynamic representations of the environment. In reality, the soil water potential will change rapidly if the plant transpiration is sufficient. Again, a dynamic link to environment will be done in the future, as we plan to integrate CPlantBox into the modelling framework CRootBox-DuMuX (Flemisch *et al.* 2011; Koch *et al.* 2018; Schnepf *et al.* 2018). By doing so, we will be able to explore the feedbacks between the plant and the environment, especially soil, in a dynamic way.

Finally, in this version of the models, carbon production is prescribed at the segment or node level. Again, this what not an issue so far, as we wanted to explore the flow distribution only. However, in the near future, we plan to include leaf-level photosynthesis module (de Pury and Farquhar 1997; Farquhar *et al.* 2001), to be able to better represent the dynamic response of the plant to its changing environment.

CONCLUSIONS

Experimental measurements of carbon and water flow can be challenging, as most available measuring methods are time-consuming and destructive (Knoblauch *et al.* 2014, 2016), preventing the continuous observation of these flow as the plant develops. Fortunately, models can be used as analysis tools for such complex experimental set-ups.

Here, we have used our coupled models (CPlantBox–PiafMunch) to reverse-estimate hidden experimental parameters. For instance, by using measured carbon flow, phloem resistance and pressure, we were able to give consistent estimates of carbon loading and unloading rate in the phloem, in the different plant organs.

More generally, this is a good example of using models as complex analysis tools. As experimental set-up and biological questions become more and more complex, it becomes harder to interpret the results. Models such as CPlantBox–PiafMunch can help integrate such results and place them into a whole-plant perspective. Carefully using the model can then give us access to additional parameters that were not available experimentally.

Exploring the interplay between the environment, the plant architecture, and the plant water and carbon flow is experimentally challenging. Measurements take time and are often destructive. However, functional structural plant models have been shown to be able to efficiently represent plant–environment interplay *in silico*.

Here, we have presented a new whole-plant framework, CPlantBox. We have shown that CPlantBox is able to represent a variety of plant architectures, both root and shoot. We also connected CPlantBox to a mechanistic model carbon and water flow, PiafMunch. The coupled model was able to reproduce realistic flow behaviour in complex plant structures. We were also able to use the models to reproduce experimental data and estimate hidden experimental variables.

MODEL AND DATA AVAILABILITY

- CPlantBox is open source under GPL 3.0 license, available at https://github.com/Plant-Root-Soil-Interactions-Modelling/CPlantBox/tree/isp/
- Model parameter files are available at: http://doi.org/10.6084/m9.figshare.9785396

- PiafMunch output of simulation example 2, 3, 4 can be found here: https://figshare.com/articles/Output_of_CPlantBox-PiafMunch_coupling/9971225
- YouTube channel of simulations: https://www.youtube.com/channel/UCPK-pFfpK94jiamgwHxX32Q

SUPPORTING INFORMATION

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

Figure S1: Fitting rst by distance to seed.

Figure S2: Schematic drawing of the 7.5 m plant.

File S1:

Table S1: Relation between loading rate, unloading rate, source phloem pressure and phloem flow rate.

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CONTRIBUTIONS BY THE AUTHORS

Writing—original draft: X.-R.Z., G.L.; writing—review and editing: J.V., A.L., H.V., G.L., X.-R.Z.; conceptualization: G.L., A.S., H.V., J.V., X.-R.Z.; software: X.-R.Z., D.L., A.L., A.S., G.L.; visualization: X.R.Z., G.L., J.V.

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CONFLICT OF INTEREST

None declared.

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