Unified representation of the C3, C4, and CAM photosynthetic pathways with the Photo3 model

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ABSTRACT

Recent interest in crassulacean acid metabolism (CAM) photosynthesis has resulted in new, physiologically based CAM models. These models show promise, yet typically are not developed with a basis that is compatible with widely used models of C3 and C4 photosynthesis. Indeed, most efforts to assess the potential of CAM still rely on empirically based environmental productivity indices, which makes uniform comparisons between CAM and non-CAM species difficult. In order to represent C3, C4, and CAM photosynthesis in a consistent, physiologically based manner, we introduce the Photo3 model. Photo3 unites a common photosynthetic and hydraulic core with components depicting the circadian rhythm of CAM photosynthesis and the carbon-concentrating mechanism of C4 photosynthesis. This work allows consistent comparisons of the three photosynthetic types for the first time. It also allows the representation of intermediate C3-CAM behavior through the adjustment of a single model parameter. Model simulations of Opuntia ficus-indica (CAM), Sorghum bicolor (C4), and Triticum aestivum (C3) capture the diurnal behavior of each species as well as the cumulative effects of long-term water limitation. These results show the model’s potential for evaluating the tradeoffs between C3, C4, and CAM photosynthesis, and for better understanding CAM productivity, ecology, and climate feedbacks.

1. Introduction

C4 photosynthesis is thought to have evolved as add-ons to the classical C3 photosynthetic pathway around 20–30 million years ago (Keeley and Rundel, 2003). Both photosynthetic processes achieve increased water use efficiency by concentrating CO2 at the site of the dark reactions of photosynthesis. Today, C4 and CAM plants fill important ecological niches in grasslands, rainforests, and arid ecosystems; C4 plants dominate in grasslands where theyaccount for almost 25% of terrestrial primary production (Still et al., 2003) whereas CAM crops make up almost 50% of plant biomass in certain arid and semi-arid regions of the world (Syvertsen et al., 1976). C4 crops such as corn (Zea mays), sugarcane (Saccharum officinarum), and sorghum (Sorghum bicolor) comprise 22% of the eighteen most common crops (Leff et al., 2004). CAM crops such as prickly pear (Opuntia ficus-indica), agave (Agave tequilana), and pineapple (Ananas comosus) are also economically significant, particularly in arid and semi-arid regions of the world.

Due to their extremely high water use efficiency and heat tolerance, the potential of CAM plants for food, fodder, and biofuel production will only become more significant as climate uncertainty and tensions over food scarcity increase (Nobel, 1991; García de Cortázar, 1992; Borland et al., 2009; Owen and Griffiths, 2014; Mason et al., 2015).

Despite the prevalence and importance of CAM plants, physiological modeling of CAM photosynthesis is well behind that of C3 and C4 photosynthesis (Farquhar et al., 1980; Von Caemmerer and Furbank, 1992). Indeed, physiological models of CAM have only recently been introduced (see e.g. Owen and Griffiths, 2013; Bartlett et al., 2014) and have not been widely adopted. Instead, Nobel’s Environmental Productivity Index (EPI), introduced in 1984, is the standard method of predicting net carbon uptake and yield for CAM plants (Nobel, 1988; Nair et al., 2012). This index, based on multiplicative indices for water, temperature and photosynthetically active radiation (PAR), is entirely empirical and does not include a physiological representation of the CAM process. Furthermore, the index is designed to be calculated at a
timescale of one month (Nobel, 1988; Owen and Griffiths, 2014), thus failing to take into account environmental variability at daily and weekly timescales, which has been shown to be an important factor in CAM functioning (Bartlett et al., 2014; Hartzell et al., 2015). This hampers the assessment of the potential impacts of CAM plants on climate, agriculture, and bioenergy production. Most climate modeling efforts include land surface models with a physiologically based representation of C3 (Rogers et al., 2017), and, often C4 photosynthesis (Cox, 2001; Cowling et al., 2007; Milly et al., 2014), but none currently include CAM photosynthesis, an important component of dryland and tropical ecosystems. The recent push for physiologically based crop modeling has also failed to take CAM crops into account. Multiple existing crop models, including 2Dleaf and MCWLA, are based on physiological models of C3 photosynthesis and stomatal conductance (Pachepsky and Acock, 1996; Tao et al., 2009), and the GECROS model supports both C3 and C4 photosynthesis based on modifications to the Farqhuar model (Yin, 2005). Despite these advances, no crop models currently exist that are capable of coherently representing the three photosynthetic types. This discrepancy propagates into the analysis of bioenergy potential. While detailed biophysical models of C3 and C4 crops enable analyses of their potential for bioenergy production (Miguez et al., 2012; Nair et al., 2012), lack of detailed CAM modeling poses a problem in better understanding its potential in this area (Yan et al., 2011; Nair et al., 2012; Owen and Griffiths, 2014; Davis et al., 2015).

The Photo3 model addresses this need by providing a consistent, physiologically based description of CAM, C3, and C4 photosynthesis coupled to environmental conditions. The model seeks to balance the complexity required to faithfully represent each process with simplicity and clarity. To achieve this, the model leverages the commonalities between the three photosynthetic types. The core of the model is based on the Rubisco-mediated carbon assimilation achieved by the light reactions and Calvin cycle of C3 photosynthesis. When representing CAM and C4 plants, this core is combined with a model for carbon fixation via phosphoenolpyruvate carboxylase (PEPC). The method for representing CAM plants is based on Bartlett et al. (2014), and adds a component for malic acid storage and release which is governed by an endogenous circadian rhythm. When representing C4 plants, a carbon concentrating mechanism based on Collatz et al., Collatz et al. (1992), Von Caemmerer and Furbank (1999), Vico and Porporato (2008) is added to the model core. The resulting integrated model allows plants of all three photosynthetic types to be simulated on a consistent basis and in a wide variety of soil and atmospheric conditions.

In this work, the model is parameterized for one representative species from each photosynthetic type: O. ficus-indica (CAM), Triticum aestivum (C3), and S. bicolor (C4). Stomatal conductance, carbon assimilation, and water use of the three species are compared at the daily and monthly scale. Finally, intermediate C3-CAM behavior is explored through the adjustment of CAM model parameters. The Photo3 model accurately captures a wide range of photosynthetic behaviors and shows promise for applications in ecological, climate, and crop modeling. Written in Python, the model is open source and publicly available on GitHub. It employs a modular structure which allows it to be easily integrated with other routines for use in a variety of applications.

Fig. 1. Photo3 model schematic. The Photo3 model is based on a core model of C3 photosynthesis with options to represent C4 photosynthesis, CAM photosynthesis, and plant water storage.
2. Materials and methods

2.1. Overview of the Photo3 model

The core of the Photo3 model, given in Section 2.2, includes the Farquhar et al. (1980) model for photosynthetic carbon demand, an optimal control model for stomatal conductance, and a model of the soil–plant–atmosphere continuum (SPAC). In the case of C4 and CAM photosynthesis, this core is coupled with a model for carbon fixation via PEPC, which is either spatially (C4) or temporally (CAM) separated from the Rubisco-mediated Calvin cycle. The SPAC model is a simple resistor-capacitor type model of the soil–plant–atmosphere continuum (e.g. Jones, 1992), and has an option to include plant water storage, which is an important feature in many succulent CAM species (Nobel, 1988). Given solar radiation, specific humidity, and temperature, the model estimates carbon assimilation and transpiration, as well as other variables of interest (see Fig. 1).

The CAM model (formulated in Section 2.3) includes all of the features of the core model and adds a representation of the carbon concentrating mechanism. Based on Bartlett et al. (2014), the diurnal rhythm of malic acid production and release is modeled through the addition of a cell vacuole, characterized by \( M \), the malic acid content, and \( z \), the circadian order variable, which represents the overall effect of gene expression, enzyme activity and/or the vacuole tonoplast in controlling the circadian rhythm. Depending on the values of \( M \) and \( z \), \( CO_2 \) may either be fixed as malic acid by PEPC and later decarboxylated and released to the Calvin cycle, or it may be directly passed to the Calvin cycle and fixed via Rubisco. To account for the CAM idling process, dark respiration stays internal to the cell and is either passed to the cell vacuole or to the Calvin cycle, depending on the light level. These differences, described in Fig. 2, allow the model to capture the unique diurnal rhythm of CAM carbon fluxes (Bartlett et al., 2014; Hartzell et al., 2015). Like the CAM model, the C4 model, presented in Section 2.4, also builds on the core Farquhar model. After the initial fixation of \( CO_2 \) into C4 acids via PEPC, which occurs in the mesophyll cell, the C4 acids are decarboxylated and the \( CO_2 \) is passed to the bundle sheath cell where it is concentrated. Within the bundle sheath cells, the Rubisco-mediated Calvin cycle fixes carbon into sugar (this process is represented using the Farquhar et al. (1980) model with the new, elevated \( CO_2 \) concentration \( c_{bs} \)). A graphical description of these carbon fluxes is given in Fig. 2.

2.2. General photosynthetic relations

The net carbon uptake is modelled as a steady-state Fickian diffusion through the stomata, i.e.,

\[ A_k = g_{k,CO_2}(c_l - c_m), \]

where \( g_{k,CO_2} \) is the stomatal conductance to \( CO_2 \), \( c_l \) is the concentration of \( CO_2 \) at the leaf surface, and \( c_m \) is the concentration of \( CO_2 \) inside the mesophyll cytosol. The stomatal conductance is assumed to scale with the square root of the vapor pressure deficit following stomatal optimization theory, an approach which agrees well with accepted empirical models (Oren et al., 1999; Hari et al., 2000; Katul et al., 2009; Medlyn et al., 2011), and can be represented as

\[ g_{k,CO_2} = \frac{a_1 A_k}{c_i \sqrt{D}}, \]

where \( a_1 \) is an empirical constant which is adjusted to account for observed differences in the \( c_{ws}/c_i \) ratio among photosynthetic types as described in Jones (1992) and \( D \) is the vapor pressure deficit.

The net photosynthetic demand for \( CO_2 \), \( A_d \), is modelled according
is the CO2 concentration at the site of the Calvin cycle, and given by

\[ \frac{\Delta}{\phi} = \frac{\Delta c}{\phi} \]

Due to the lack of temporal separation of CO2 uptake and assimilation in C3 and C4 photosynthesis, the net carbon uptake \( A_d \) is equal to the net photosynthetic demand \( A_d \) for these photosynthetic types. The relationship between \( A_n \) and \( A_d \) for CAM includes a temporal separation and is described in Section 2.3. The carbon demand \( A_{\phi, c, T}(\phi, c, T) \) is given by

\[ A_{\phi, c, T}(\phi, c, T) = \min[A_n(c, T), A_d(\phi, c, T)] \]

where \( A_n(c, T) \) is the Rubisco-limited photosynthetic rate, \( A_d(\phi, c, T) \) is the light-limited photosynthetic rate, \( T \) is the leaf temperature, \( c_s \) is the CO2 concentration at the site of the Calvin cycle, and \( \phi \) is the incoming solar radiation (see Appendix A for details). The relevant CO2 concentration \( c_s \) varies based on the photosynthetic type. For C3 plants, \( c_s \) is the mesophyll concentration \( c_{m0} \); and for CAM plants, it is either \( c_s \) or the corrected mesophyll CO2 concentration \( c_c \) (when malic acid is being decarboxylated), the mesophyll CO2 concentration is corrected to account for the elevated CO2 concentration as \( c_c = c_m(c_m D) + c_{m0}(z, M) \) following Bartlett et al. (2014).

The effects of water stress reduce the photosynthetic demand according to a ‘vulnerability’ function of the leaf water potential, \( f_b(\psi) \), here represented for simplicity as a piecewise linear function which decreases between the point of onset of water stress, \( \psi_{IA1} \), and the point of stomatal closure \( \psi_{IAD} \), i.e.,

\[ f_b(\psi) = \begin{cases} 0, & \psi < \psi_{IA1} \\ \frac{(\psi_{IA1} - \psi_{IAD})(\psi - \psi_{IA1})}{(\psi_{IA1} - \psi_{IAD})}, & \psi_{IA1} < \psi \leq \psi_{IA1} \\ 1, & \psi > \psi_{IA1} \end{cases} \]

where the leaf water potentials \( \psi_{IA1} \) and \( \psi_{IAD} \) are species-dependent (see Table 1). This piecewise function, also used in Daly et al. (2004), provides results similar to other response functions commonly used in describing plant response to water stress, such as sigmoidal curves.

Table 1: Plant photosynthetic parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>O. ficus-indica</th>
<th>S. bicolor</th>
<th>T. aestivum</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a_1 )</td>
<td>2.08&lt;sup&gt;b&lt;/sup&gt;</td>
<td>1.73&lt;sup&gt;b&lt;/sup&gt;</td>
<td>3.46&lt;sup&gt;c&lt;/sup&gt;</td>
<td>( \mu mol ) mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Stomatal conductance coefficient, Eq. (2)</td>
</tr>
<tr>
<td>( k_0 )</td>
<td>302&lt;sup&gt;+&lt;/sup&gt;</td>
<td>302</td>
<td>302</td>
<td>( \mu mol ) mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Michaelis constant for CO2 at ( T_s )</td>
</tr>
<tr>
<td>( k_0 )</td>
<td>1.73&lt;sup&gt;d&lt;/sup&gt;</td>
<td>256</td>
<td>256</td>
<td>( \mu mol ) mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Michaelis constant for O2 at ( T_s )</td>
</tr>
<tr>
<td>( H_k )</td>
<td>59,430&lt;sup&gt;e&lt;/sup&gt;</td>
<td>59,430</td>
<td>59,430</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Activation energy for ( k_e )</td>
</tr>
<tr>
<td>( H_k )</td>
<td>36,000&lt;sup&gt;f&lt;/sup&gt;</td>
<td>36,000</td>
<td>36,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Activation energy for ( k_c )</td>
</tr>
<tr>
<td>( R_0 )</td>
<td>0.32&lt;sup&gt;g&lt;/sup&gt;</td>
<td>0.32</td>
<td>4.93&lt;sup&gt;h&lt;/sup&gt;</td>
<td>( \mu mol ) m&lt;sup&gt;-2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Standard dark respiration at 25 C</td>
</tr>
<tr>
<td>( R_0 )</td>
<td>53,000&lt;sup&gt;i&lt;/sup&gt;</td>
<td>53,000</td>
<td>53,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Activation energy for ( R_0 )</td>
</tr>
<tr>
<td>( c_2 )</td>
<td>0.3&lt;sup&gt;j&lt;/sup&gt;</td>
<td>3</td>
<td>3</td>
<td>( \mu mol ) CO2 mol&lt;sup&gt;-1&lt;/sup&gt; photons</td>
<td>Quantum yield of photosynthesis, Eq. (A.7)</td>
</tr>
<tr>
<td>( V_{C_m} )</td>
<td>13&lt;sup&gt;k&lt;/sup&gt;</td>
<td>39&lt;sup&gt;l&lt;/sup&gt;</td>
<td>107.4&lt;sup&gt;l&lt;/sup&gt;</td>
<td>( \mu mol ) m&lt;sup&gt;-2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Maximum carboxylation rate</td>
</tr>
<tr>
<td>( A_{\phi} )</td>
<td>72,000&lt;sup&gt;m&lt;/sup&gt;</td>
<td>72,000</td>
<td>62,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Activation energy for ( V_{C_m} )</td>
</tr>
<tr>
<td>( h_{\phi} )</td>
<td>200,000&lt;sup&gt;n&lt;/sup&gt;</td>
<td>200,000</td>
<td>202,900&lt;sup&gt;o&lt;/sup&gt;</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Decrease inactivation energy for ( h_{\phi} )</td>
</tr>
<tr>
<td>( \delta_{\psi} )</td>
<td>26</td>
<td>180&lt;sup&gt;p&lt;/sup&gt;</td>
<td>184.9&lt;sup&gt;q&lt;/sup&gt;</td>
<td>( \mu mol ) m&lt;sup&gt;-2&lt;/sup&gt;s&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Electron transport rate, Eq. (A.6)</td>
</tr>
<tr>
<td>( \delta_{\phi} )</td>
<td>50,000&lt;sup&gt;r&lt;/sup&gt;</td>
<td>50,000</td>
<td>50,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Activation energy for ( J_{\max} )</td>
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<tr>
<td>( \delta_{\psi} )</td>
<td>200,000&lt;sup&gt;s&lt;/sup&gt;</td>
<td>200,000</td>
<td>200,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>Oxygen concentration</td>
</tr>
<tr>
<td>( \gamma_{A1} )</td>
<td>0.05&lt;sup&gt;t&lt;/sup&gt;</td>
<td>0.5&lt;sup&gt;u&lt;/sup&gt;</td>
<td>0.5&lt;sup&gt;u&lt;/sup&gt;</td>
<td>MPa</td>
<td>Entropy term for carboxylation</td>
</tr>
<tr>
<td>( \gamma_{A0} )</td>
<td>2 s</td>
<td>2 s</td>
<td>2 s</td>
<td></td>
<td>Entropy term for electron transport</td>
</tr>
<tr>
<td>( \gamma_{A1} )</td>
<td>1K</td>
<td>1K</td>
<td>1K</td>
<td></td>
<td>Reference temperature</td>
</tr>
<tr>
<td>( \gamma_{A0} )</td>
<td>53,000&lt;sup&gt;v&lt;/sup&gt;</td>
<td>53,000</td>
<td>53,000</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>CO2 compensation point at ( T_s ), Eq. (A.3)</td>
</tr>
<tr>
<td>( \gamma_{A1} )</td>
<td>1K</td>
<td>1K</td>
<td>1K</td>
<td></td>
<td>CO2 compensation point at ( T_s ), Eq. (A.3)</td>
</tr>
<tr>
<td>( \gamma_{A0} )</td>
<td>59,430&lt;sup&gt;w&lt;/sup&gt;</td>
<td>59,430</td>
<td>59,430</td>
<td>J mol&lt;sup&gt;-1&lt;/sup&gt;</td>
<td>CO2 compensation point at ( T_s ), Eq. (A.3)</td>
</tr>
<tr>
<td>( \gamma_{A1} )</td>
<td>1K</td>
<td>1K</td>
<td>1K</td>
<td></td>
<td>CO2 compensation point at ( T_s ), Eq. (A.3)</td>
</tr>
</tbody>
</table>

<sup>a</sup> Based on Leuning (1995).
<sup>b</sup> Based on Jones (1992).
<sup>c</sup> Based on Sun et al. (2015).
<sup>d</sup> Based on Long et al. (1993).
<sup>e</sup> Based on Nobel and Hartsock (1983), Cui et al. (1993), Pimienta-Barrios et al. (2000).
<sup>f</sup> Based on Collatz et al. (1992).
<sup>g</sup> Based on Kattge and Knorr (2007).
<sup>h</sup> Based on Daly et al. (2004).
<sup>i</sup> Based on Barthet et al. (2014).
<sup>j</sup> Based on Contour-Ansel et al. (1996).
<sup>k</sup> Based on Siddique et al. (2000).
The dark respiration, $R_d$, is typically a small fraction of the carbon assimilation, its inclusion is optional except in the case of CAM where it is an important component of CAM idling behavior during periods of extended stomatal closure. Here it is represented as a temperature-dependent process according to a modified Arrhenius equation (see Appendix A).

### 2.3. CAM-specific relations

In the CAM model, a carbon pool is added to represent malic acid uptake and release from the cell vacuole (see Fig. 2). The net flux of carbon through the stomata, $A_n$, is comprised of a flux from the stomata to the Calvin cycle, $A_{av}$, and one to the cell vacuole, $A_{sv}$, i.e.,

$$A_n = A_{av} + A_{sv}.$$

(6)

where $z$ and $M$ are the circadian rhythm order variable and the malic acid concentration, respectively (described below), and the fluxes $A_{av}$ and $A_{sv}$ are related to the carbon demand $A_d$ through the circadian state as described in Appendix C. The dark respiration flux, $R_d$, is likewise divided into a flux to the vacuole, $R_{sv}$, and one to the Calvin cycle, $R_{av}$. Carbon is stored in the cell vacuole as malic acid and is released from the vacuole as the flux $A_{sv}$. The diurnal cycle of uptake and release from the vacuole, which governs the fluxes to and from the vacuole, is represented by a pair of balance equations for $M$, the malic acid concentration, and $z$, the circadian rhythm order. The balance equation for the malic acid concentration is given by

$$\frac{dM}{dt} = \frac{M_{\text{max}}}{\alpha} \left( \frac{\beta(z) - \mu}{\beta(z) - \mu} + 1 \right) \left( e^{-t/\tau} - \frac{\beta(z) - \mu}{\beta(z) - \mu} - c_2 \right) + \left( 1 - f_0(z) \right), \quad \text{for } z \leq 0$$

$$\frac{dM}{dt} = \frac{M_{\text{max}}}{\alpha} \left( \frac{\beta(z) - \mu}{\beta(z) - \mu} + 1 \right) \left( e^{-t/\tau} - \frac{\beta(z) - \mu}{\beta(z) - \mu} - c_2 \right), \quad \text{for } z > 0 ,$$

(9)

where $T_h$ and $T_l$ are the high and low temperature values for the circadian rhythm, and $c_1$, $c_2$, $\mu$, and $\beta$ are circadian oscillator constants included in Table 2. This formulation follows Bartlett et al. (2014) with the addition of the term $1 - f_0(z)$ which synchronizes the circadian rhythm with the prevailing light cycle (this new term increases $M_{\text{max}}$ at high $z$ values during the night, ensuring that the uptake of malic acid continues at night even if the previous day’s cycle has not completely depleted the store of malic acid). The formulations of the model fluxes are given in Appendix C. These adjustments to the functions given in Bartlett et al. (2014) improve model robustness to highly variable environmental inputs.

### 2.4. C4-specific relations

In the C4 plant, the influx of CO$_2$ to the bundle sheath cell is driven by the C4 pump and is modeled by a Michaelis-Menten type dependence on the mesophyll cytosol CO$_2$ concentration, $c_m$ as in Von Caemmerer, Von Caemmerer (2000), Vico and Porporato (2008) (see Fig. 2). The PEP regeneration rate, $V_{pr}$, is bounded by the upper limit $V_{pr}$, i.e.,

$$V_F(c_m) = \min \left( \frac{c_m V_{pr,\text{max}}}{c_m + K_p}, V_T \right),$$

(10)

where $V_{pr,\text{max}}$ is the maximum PEP carboxylation rate and $K_p$ is the Michaelis-Menten coefficient. Leakage of CO$_2$ from the bundle sheath cell is modelled as a diffusion flux from the bundle sheath to the leaf via the stomata.

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**Table 2**: CAM photosynthetic parameters (based on Opuntia ficus-indica).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$</td>
<td>0.365</td>
<td></td>
<td>Circadian oscillator constant</td>
</tr>
<tr>
<td>$c_2$</td>
<td>0.555</td>
<td></td>
<td>Circadian oscillator constant</td>
</tr>
<tr>
<td>$c_3$</td>
<td>10^4</td>
<td></td>
<td>Circadian oscillator constant</td>
</tr>
<tr>
<td>$\mu$</td>
<td>0.5</td>
<td></td>
<td>Circadian oscillator constant</td>
</tr>
<tr>
<td>$\beta$</td>
<td>2.764</td>
<td></td>
<td>Circadian oscillator constant</td>
</tr>
<tr>
<td>$M_{\text{max}}$</td>
<td>190</td>
<td>mol m$^{-3}$</td>
<td>Maximum malic acid concentration</td>
</tr>
<tr>
<td>$A_{\text{max}}$</td>
<td>13.5</td>
<td>mol mol$^{-1}$/s</td>
<td>Maximum rate of malic acid storage</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>1/100</td>
<td>min</td>
<td>Relaxation time</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>1/7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$k$</td>
<td>0.003</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$T_{av}$</td>
<td>288.65</td>
<td>K</td>
<td></td>
</tr>
<tr>
<td>$T_H$</td>
<td>302.65</td>
<td>K</td>
<td></td>
</tr>
<tr>
<td>$T_L$</td>
<td>283.15</td>
<td>K</td>
<td></td>
</tr>
<tr>
<td>$c_v$</td>
<td>3000</td>
<td>mol mol$^{-1}$/s</td>
<td>Parameter for decarboxylation of malic acid</td>
</tr>
</tbody>
</table>

---

**Table 3**: C4 photosynthetic parameters (based on Sorghum bicolor).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b_m$</td>
<td>0.013</td>
<td>mol/m$^{-2}$/s</td>
<td>Conductance between bundle sheath and mesophyll</td>
</tr>
<tr>
<td>$V_{pr,\text{max}}$</td>
<td>120</td>
<td>mol mol$^{-1}$/s</td>
<td>Maximum PEP carboxylation rate</td>
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<tr>
<td>$V_{pr}$</td>
<td>80</td>
<td>mol mol$^{-1}$/s</td>
<td>PEP regeneration rate</td>
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<tr>
<td>$K_p$</td>
<td>80</td>
<td>mol mol$^{-1}$</td>
<td>Michaelis-Menten coefficient for C4</td>
</tr>
</tbody>
</table>

---

* Based on Bartlett et al. (2014).
mesophyll cell, i.e.,
$$L_{bs}(c_{bs}, c_m) = L_{bs}(c_{bs} - c_m),$$  (11)
where $g_{bs}$ is the conductance between the bundle sheath and mesophyll cells and $c_{bs}$ is the CO$_2$ concentration in the bundle sheath cells. Finally, we introduce a balance equation for the CO$_2$ fluxes into and out of the bundle sheath cell, i.e.,
$$V_P(c_m) = A_L(\phi, c_{bs}, T_l, \psi_l) + L_{bs}(c_{bs}, c_m),$$  (12)
and solve for the CO$_2$ concentration in the bundle sheath cell, $c_{bs}$, by combining Eq. (12) with Eqs. (10) and (11). The carbon assimilation is then calculated according to Eq. (3). Parameters for the C4 model are included in Table 3.

2.5. Plant hydraulics and capacitance

The transpiration flux, $E$, is driven by the difference between the specific humidity internal to the leaf and that of the atmosphere, i.e.,
$$E = \frac{g_{sa}\rho}{\rho_w}[q_i(T_l, \psi_l) - q_a].$$  (13)
where $g_{sa}$ is the series of the atmospheric conductance and the combined stomatal-cuticular conductance (see Appendix B), $\rho$ is the density of air, $\rho_w$ is the density of water, $q_i$ is the specific humidity internal to the leaf, and $q_a$ is the specific humidity of the atmosphere. At the same time, the transpiration flux must be equal to the flux of water through the plant, i.e.,
$$E = g_{srp}(\psi_s - \psi_l).$$  (14)
where $g_{srp}$ is the series of the soil-root and plant conductances (see Appendix B), $\psi_s$ is the soil water potential, and $\psi_l$ is the leaf water potential. These relations are joined by the equation for energy balance, which equates the incoming heat flux to the outgoing sensible and latent heat fluxes, i.e.,
$$\phi g_a = \lambda \rho c_T T_a = - E.$$

Table 4

Plant hydraulic parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>O. ficus-indica</th>
<th>S. bicolor</th>
<th>T. aestivum</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_{max}$</td>
<td>0.04$^a$</td>
<td>0.13$^i$</td>
<td>11.7$^d$</td>
<td>$\mu$m MPa$^{-1}$ s$^{-1}$</td>
<td>Maximum xylem conductance per unit leaf area</td>
</tr>
<tr>
<td>LAI</td>
<td>3$^b$</td>
<td>5$^j$</td>
<td>5$^o$</td>
<td>m$^2$ m$^{-2}$</td>
<td>Leaf area per unit ground area</td>
</tr>
<tr>
<td>$Z_r$</td>
<td>0.1$^c$</td>
<td>0.5$^k$</td>
<td>0.75$^p$</td>
<td>m</td>
<td>Mean rooting depth</td>
</tr>
<tr>
<td>$k_{AR}$</td>
<td>3$^e$</td>
<td>5.6$^l$</td>
<td>5.6$^l$</td>
<td>mm$^2$ m$^{-2}$</td>
<td>Root area index under well watered conditions</td>
</tr>
<tr>
<td>$d$</td>
<td>8$^m$</td>
<td>8$^m$</td>
<td>8$^m$</td>
<td>Parameter accounting for root growth</td>
<td></td>
</tr>
<tr>
<td>$c_{2a}$</td>
<td>1$^n$</td>
<td>2.65$^o$</td>
<td>1.65$^o$</td>
<td>mol/m$^2$s</td>
<td>Ratio of $g_{sa,CO_2}$ to $g_{sa,CO_2}$</td>
</tr>
<tr>
<td>$E_{cut}$</td>
<td>0$^q$</td>
<td>0.1802$^{qs}$</td>
<td>0.3$^q$</td>
<td>mm/s</td>
<td>Cuticular conductance per unit leaf area</td>
</tr>
<tr>
<td>$g_{w}$</td>
<td>324$^r$</td>
<td>61$^s$</td>
<td>61$^s$</td>
<td>mm/s</td>
<td>Atmospheric conductance per unit ground area</td>
</tr>
<tr>
<td>$Z_w$</td>
<td>0.00415$^t$</td>
<td>–</td>
<td>–</td>
<td>Parameter for Eq. (B.6)</td>
<td></td>
</tr>
<tr>
<td>$g_{w,CO_2}$</td>
<td>0.002$^u$</td>
<td>–</td>
<td>–</td>
<td>$\mu$m MPa$^{-1}$ s$^{-1}$</td>
<td>Maximum conductance between stored water and transport pathway, per unit leaf area</td>
</tr>
<tr>
<td>$h$</td>
<td>2$^v$</td>
<td>–</td>
<td>–</td>
<td>Parameter for Eq. (B.6)</td>
<td></td>
</tr>
<tr>
<td>$j$</td>
<td>2$^v$</td>
<td>–</td>
<td>–</td>
<td>Parameter for Eq. (B.6)</td>
<td></td>
</tr>
<tr>
<td>$m$</td>
<td>4$^v$</td>
<td>–</td>
<td>–</td>
<td>Parameter for Eq. (B.7)</td>
<td></td>
</tr>
<tr>
<td>$c$</td>
<td>0.27$^w$</td>
<td>–</td>
<td>–</td>
<td>MPa$^{-1}$</td>
<td>Intrinsic plant hydraulic capacitance, Eq. (B.2)</td>
</tr>
<tr>
<td>$f$</td>
<td>0.5</td>
<td>–</td>
<td>–</td>
<td>Fractional height of hydraulic capacitance</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Estimated from a succulent CAM species based on Bartlett et al. (2014).
$^b$ Based on Nobel (1988).
$^c$ Based on Snyman (2005).
$^d$ Based on Daly et al. (2004).
$^e$ Based on Flexas et al. (2008).
$^f$ Based on Jones (1992) for a wind speed of 2 m/s at 2 m altitude, with a plant height of 2 m.
$^g$ Based on Goldstein et al. (1991).
$^h$ Based on Kocacinar and Sage (2003).
$^i$ Based on Olufayo et al. (1996).
$^j$ Based on Bremner and Preston (1986).
$^k$ Based on Vico and Porporato (2008).
$^l$ Based on Muchow and Sinclair (1989).
$^m$ Based on Kocacinar and Sage (2003).
$^n$ Based on Olufayo et al. (1996).
$^o$ Based on Bremner and Preston (1986).
$^p$ Based on Vico and Porporato (2008).
$^q$ Based on Muchow and Sinclair (1989).
$^r$ Based on Jones (1992) for a wind speed of 2 m/s at 2 m altitude, with a plant height of 1 m.
$^s$ Based on Lunagaria and Shekh (2006).
$^t$ Based on Bandyopadhyay et al. (2003).
$^u$ Based on Kerstiis (1996).
Table 5
Soil parameters.a

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Loamy sand</th>
<th>Sandy loam</th>
<th>Loam</th>
<th>Clay</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_s$ (cm d$^{-1}$)</td>
<td>100</td>
<td>80</td>
<td>20</td>
<td>1</td>
</tr>
<tr>
<td>$S_r$ (MPa)</td>
<td>$-1.7 \times 10^{-4}$</td>
<td>$-7.0 \times 10^{-4}$</td>
<td>$-1.43 \times 10^{-3}$</td>
<td>$-1.82 \times 10^{-3}$</td>
</tr>
<tr>
<td>$b$</td>
<td>4.38</td>
<td>4.9</td>
<td>5.39</td>
<td>11.4</td>
</tr>
<tr>
<td>$n$</td>
<td>0.42</td>
<td>0.43</td>
<td>0.45</td>
<td>0.5</td>
</tr>
<tr>
<td>$n_t$</td>
<td>0.08</td>
<td>0.14</td>
<td>0.19</td>
<td>0.47</td>
</tr>
</tbody>
</table>

a Parameters from Rodriguez-Iturbe and Porporato (2004).

conductance, $c_p$, is the specific heat of air, $T_o$ is the atmospheric temperature, and $\lambda_w$ is the latent heat of vaporization. Eqs. (13)–(15) are solved simultaneously for the three unknowns: the transpiration $E$, the leaf temperature $T_L$, and the leaf water potential $\psi_c$.

Plant water storage is included as an option in the model. While it is generally negligible for most C3 and C4 crops, plant water storage significantly affects water stress and carbon assimilation for plants with a substantial water storage capacity, including most CAM plants. Therefore, we include plant water storage when modeling CAM plants in this study, but not when modeling C3 and C4 plants. Plant water storage is represented in this model as a simple capacitor located at a height which is a fraction $f$ of the total plant height as in Hartzell et al. (2017) (see Fig. 3 and Appendix B). Using this scheme, the change in the plant relative water content $w$ is given by the balance equation

$$ \frac{dLAI}{dt} \cdot w = q_w(s, w) - E, $$

where $Z_w$ is the total available water storage depth of the plant on a leaf area basis, LAI is the leaf area index, and $s$ is the soil moisture. The transpiration flux $E$ is now given by the sum of the fluxes from the soil, $q_s$, and the plant water storage, $q_w$, such that

$$ E = q_s + q_w = E_{soil}(\psi_c - \psi_{gw}) + E_{sw}LAI(\psi_{gw} - \psi_t). $$

where $\psi_w$ is the water potential at the storage connection node, $E_{soil}$ is the conductance between the soil and storage connection node, $g_{soil}$ is the conductance between the site of water storage and the storage connection node, and $\psi_t$ is the water potential of the water storage tissue (see Appendix B and Table 4 for details). The addition of plant water storage adds a fourth unknown ($\psi_w$) to the water balance, which may now be formulated as described in Appendix B.

The soil moisture may either be provided as a model input or determined through the balance equation,

$$ \frac{dZ_w}{dt} = -q_w(s, w) - L(s) - E(s) + R(t), $$

where $n$ is the soil porosity, $Z_w$ is the rooting depth and $s$ is the volumetric soil moisture averaged over the rooting depth. Total losses from the soil are due to plant water uptake $q_s(s, w)$, leakage loss $L(s)$, and evaporation $E(s)$ (see Rodriguez-Iturbe and Porporato (2004) for details). In Eq. (18), the rainfall $R(t)$ may be specified either as a model input or may be generated within the model as a stochastic process which requires the mean rainfall depth and frequency as input parameters. Currently a range of soil types are represented by the four soil options included in the model: loamy sand, sandy loam, loam, and clay. Soil parameters are included in Table 5.

2.6. Model implementation

Environmental inputs for the model are solar radiation, air temperature, specific humidity, soil moisture, and soil type. Because of the strong dependence of CAM photosynthesis on variability in environmental conditions at the sub-daily scale, the model operates with a 30-minute timestep. Solar radiation, specific humidity, and air temperature data with an hourly timescale may be interpolated to give values at each model timestep. Alternatively, values for these variables may be generated internally to the model using a built-in boundary-layer simulation following the approach presented in Daly et al. (2004). Values for soil moisture may be provided at each model timestep, may be generated by the model from user provided rainfall data, or may be generated internally by the model given certain assumptions, i.e. constant soil moisture, drydown conditions, or stochastic rainfall generation. The model is currently parameterized with hydraulic and photosynthetic properties for three representative species, T. aestivum (C3), S. bicolor (C4), and O. ficus-indica (CAM) (see Tables 1–4); these species were selected because they are among the most well-studied and economically important species of each photosynthetic group (Leff et al., 2004; Paterson et al., 2008). These properties are meant to represent plants at the mature stage in the growing season, and are assumed to be approximately constant over the model duration.

2.7. Model validation and testing

2.7.1. Model validation

The model was validated using data collected under both well-watered and droughted conditions for the three representative crops (see Section 3.1). Model results under well-watered conditions for O. ficus-indica were compared to results from a 24-h laboratory experiment undertaken by Nobel and Hartsook (1983) with 12 h of light and 12 h of darkness. In this simulation, the day period was characterized by a solar radiation of 244 W/m$^2$, a temperature of 25 C, and a relative humidity of 40%, while the night period was characterized by a temperature of 15 C and a relative humidity of 60% according to the conditions present in the laboratory experiment. To facilitate comparisons of model performance with experimental data for S. bicolor and T. aestivum, the model was forced with typical non-limiting laboratory conditions of 12 h light:12 h darkness with a solar radiation of 391 W/m$^2$ during the light period, a constant temperature of 26 C, constant relative humidity of 80%, and 0.7 volumetric soil moisture in loam soil. To enable comparison of model results with data for O. ficus-indica, the model was run for a 40 day drydown in loamy sand with solar radiation, temperature, and relative humidity obtained from the National Solar Radiation Database (NSRDB) (National Renewable Energy Laboratory, 2017) on March 17, 2015 at a weather station nearby the study location in Til Til, Chile. Results were compared with data from Acevedo et al. (1983) describing carbon assimilation and stomatal conductance of under water-stressed conditions.

2.7.2. Diurnal dynamics

The diurnal dynamics of the three photosynthetic types were compared under typical, well-watered, growing conditions (see Section 3.2). The model was run using meteorological data from Temple, TX on April 1, 2015, imposing a soil moisture of 0.5 and a soil type of sandy loam. The solar radiation, air temperature, and specific humidity for the site were obtained from the NSRDB data viewer (National Renewable Energy Laboratory, 2017).

2.7.3. Long-term performance under drought

We evaluated the relative long-term performance of the three crops during a drought (Section 3.3) by simulating a drydown of 40 days was simulated beginning with a volumetric soil moisture of 0.5 and using temperature, relative humidity, and solar radiation data from Temple TX from April 1, 2015 until May 10, 2015 (National Renewable Energy Laboratory, 2017). During the drydown, the soil moisture was calculated according to Eq. (18).

2.7.4. Representation of C3-CAM intermediates

To test the ability of the model to capture C3/CAM intermediate photosynthetic types, the model was executed with various levels of maximum malic acid storage capacity, $M_{max}$ (see Section 3.4). Values tested were $M_{max} = 190$ mol/m$^3$ (default model setting), 95 mol/m$^3$
(50% of the default setting), and 1.9 mol/m³ (1% of the default setting). Results from these simulations were compared to a simulation run with all the photosynthetic parameters of *O. ficus-indica*, but with the photosynthetic type set equal to C3 rather than CAM. For consistency, plant water storage and respiration were not included in any of these simulations. Simulations were run for sandy loam soil with a constant soil moisture of 0.5 and weather conditions found in Temple, TX on April 3, 2015 (National Renewable Energy Laboratory, 2017).

3. Results and discussion

3.1. Model validation

For *O. ficus-indica*, the magnitude and diurnal dynamics of both carbon assimilation (see Fig. 4a) and stomatal conductance (data not shown) closely match those observed in controlled laboratory experiments. Carbon assimilation reaches a maximal value of 10 μmol/m²/s, in agreement with the data, and stomatal conductance reaches a maximal value of 3.0 mm/s, as compared with the observed maximal value of 2.8 mm/s. The diurnal dynamics show a relatively good fit, with a slight underestimate of carbon assimilation in the middle of the night (hours 21–1) and a slight overestimate of carbon assimilation at dawn (hour 6). At dusk, the timing of the onset of CAM carbon assimilation matches very well with the data, while the decrease in carbon assimilation and stomatal conductance at dawn is slightly slower than that observed. For *S. bicolor*, the carbon assimilation rate under optimal conditions is 48 μmol/m²/s, which lies within the range of published experimental ranges of 34–48 μmol/m²/s (Peng, 1990) and 40 μmol/m²/s (Resende et al., 2012) (see Fig. 4e). For *T. aestivum*, the maximal simulated carbon assimilation rate is 28 μmol/m²/s, which agrees well with experimental values of 24–29 μmol/m²/s (Evans, 1983) and 32 μmol/m²/s (Martin and Ruiz-Torres Na, 1992) (see Fig. 4e).

Model responses to water limitations also compare well with data for the three representative species. Fig. 4b shows daily stomatal conductance for *O. ficus-indica* at various levels of soil water potential simulated during a drydown. The daily maximal stomatal conductance decreases from a maximum under well-watered conditions to 50% of its initial value at a soil water potential of approximately -0.7 MPa. This behavior is a good fit with field measurements of stomatal conductance taken during a progressive drydown (Acevedo et al., 1983). Finally, the model response to water limitation $f_s(\psi_l)$, given by Eq. (5), is compared with experimental data for carbon assimilation at a range of leaf water potentials for both *S. bicolor* and *T. aestivum*. Data shown include two cultivars of *S. bicolor*: ICSV 1063 and MIGSOR (data from Contour-Ansel et al., 1996), and several cultivars of *T. aestivum: Kanchan, Sonalika, Kalyansona, and C306* (data from Siddique et al. (2000) (circles), data for TAM W-101 (Johnson et al., 1987) (squares), and data for TAM W-101 and Sturdy (Martin and Ruiz-Torres Na, 1992) (triangles).

3.2. Diurnal dynamics

Due to its detailed representation of CAM dynamics, the Photo3 model is able to compare CAM, C3, and C4 functioning at a half-hourly
timescale. Fig. 5a shows the solar radiation, air temperature, and specific humidity for a typical April day in Temple, TX. Model responses of carbon assimilation, transpiration, and stomatal conductance for each of the photosynthetic types are shown in Fig. 5b–d. The characteristic stomatal behavior of CAM is clearly shown, with stomata opening primarily at night. A combination of a low stomatal conductance and a low nocturnal driving force for transpiration during this period result in a very low transpiration with a moderate nocturnal carbon assimilation. The carbon concentrating behavior of C4 results in a high maximum carbon assimilation, while the stomatal conductance and transpiration are slightly lower than that of C3. Under these conditions, the C4 plant shows a high productivity and a high water use efficiency, while the CAM plant shows a relatively low productivity but a very high water use efficiency.

3.3. Long-term performance under drought

Model simulations of cumulative carbon assimilation and water use during a drought period are shown in Fig. 6 for the three photosynthetic types. While the C3 and C4 crops initially have high productivity, assimilating carbon at a rate two to three times that of the CAM crop, the productivity of the C3 and C4 crops undergoes a large decrease after about 8–10 days as the soil dries to below 0.3 volumetric soil moisture (Fig. 6a). Meanwhile, the CAM crop exhibits a slower, but more persistent rate of carbon gain. By day 22, the total carbon assimilation of O. ficus-indica surpasses that of T. aestivum, and by day 29, it surpasses that of S. bicolor. The CAM crop also shows a much lower cumulative transpiration, by a factor of nearly five, during the early stages of the drought, while the overall water use of the C3 and C4 crops are similar during this period (see Fig. 6b). This means that the soil in the CAM simulation remains at a much higher moislevel for the first 20 days of
the simulation (see Fig. 6c). While the CAM species exhibits a lower productivity under non-water-limited conditions, it exhibits a much higher water use efficiency and its productivity persists longer under water-limited conditions. After a 40-day drydown, the CAM crop ultimately assimilates twice as much carbon as the C3 species and 50% more than the C4 species. At the same time, its total transpiration is less than half that of the C3 species and about 70% that of the C4 species. Depending on the specific environmental conditions, the photosynthetic water use efficiency of CAM is two to six times higher than C3, and one to five times higher than C4 (Fig. 6d). This consistent basis of comparison, which incorporates the effects of environmental variability at both long and short timescales, allows the model user to quantify the costs and benefits of crops with different photosynthetic types in water-limited ecosystems.

3.4. Representation of C3-CAM intermediates

CAM photosynthesis is generally not a discrete trait, rather, a spectrum of C3-CAM behavior exists in nature (Winter et al., 2015; Bräutigam et al., 2017). Metabolite fluxes similar to CAM fluxes have been shown in C3 plants, to a much smaller degree (Winter et al., 2015; Bräutigam et al., 2017), and some CAM plants, including *O. ficus-indica*, *Agave deserti*, and *Mesembryanthemum crystallinum* show dramatic changes in the level of CAM expression throughout their lifespan, switching from C3 to CAM photosynthesis during the process of development or in response to water stress (Kluge and Ting, 1978; Winter et al., 1978, 2008; Jordan and Nobel, 1979; Acevedo et al., 1983; Winter and Holtum, 2011). The consistent formulations of the three different photosynthetic pathways in the Photo3 model allows intermediate CAM-C3 behavior to be explored through the adjustment of a single model parameter. This is the first time that such an analysis has been possible in a model coupled to the soil–plant–atmosphere continuum.

As CAM expression becomes stronger, vacuole size and maximum malic acid storage capacity increase. Indeed, maximum malic acid content is a typical measure of the strength of CAM expression (Kluge and Ting, 1978). By altering the maximum malic acid concentration \( M_{\text{mal}} \) in the CAM model, C3 behavior can be retrieved from the CAM model framework. These results are shown in Fig. 7a–c, which shows carbon assimilation, transpiration, and stomatal conductance for *Opuntia ficus-indica* with a constant soil moisture of 0.5 and weather conditions found in Temple, TX on April 3, 2015.

As the maximum malic acid concentration approaches zero, the length of nocturnal stomatal opening becomes shorter until it approaches zero in accordance with the C3 model. Meanwhile, the stomata begin to open for increasingly longer periods during the day. For very low values of maximum malic acid concentration, the stomatal conductance,
carbon assimilation, and transpiration of the CAM model match those of the C3 model.

The relevant CAM fluxes $A_{co2}$, $A_{oci}$, and $A_{c}$ are shown in Fig. 7d-f for various levels of CAM expression. As $M_{max}$ decreases, the fluxes $A_{co2}$ and $A_{oci}$ decrease while the duration of $A_{c}$ increases until it is occurring for all daylight hours as $M_{max}$ approaches zero. This behavior can be understood by referring to Appendix C. As $M_{max}$ decreases, the amount of malic acid stored during the night becomes smaller, and the malic acid is more quickly depleted during the day. As a result, the carbon function $f_{c}$, which depends on the malic acid concentration (see Eq. (C.3)) is at a non-zero value for a briefer period after the onset of light. As $f_{c}$ approaches zero during the day, $A_{ oci}$ approaches zero and $A_{c}$ approaches $A_{c}$, yielding C3-like behavior (see Eqs. (C.9) and (C.1)). Likewise, the flux $A_{oci}$ is restricted to smaller time increments at dawn and dusk and finally approaches zero according to Eq. (C.5).

4. Conclusions

Results of the Photo3 model allow the comparison of CAM, C3, and C4 species in a consistent framework. This detailed model is streamlined, user-friendly, and robust to a wide range of environmental conditions. Thus, it is ready to be included as a component of earth system models, crop models, and bioenery models. In each of these areas, a more detailed representation of CAM functioning can illuminate important questions. The inclusion of C4 plants in earth system models has been evaluated and has been shown to have a significant effect on land cover and on local climate conditions (Cowling et al., 2007). Thus, CAM plants, which arguably inhabit more extreme climates, may also be expected to show important local effects. A more detailed representation of CAM in crop modeling will be a useful tool for evaluating potential productivity, planting strategies, and water use strategies for CAM agriculture. The open source, modular nature of the model is designed for to be user friendly and easy to couple with existing modeling efforts. Photo3 shows promise for use in a variety of research applications where models of CAM photosynthesis are currently lacking, including the prediction of CAM climate feedbacks, productivity, and biofuel potential.

Software availability

The Photo3 software can be accessed for free at https://samhartz.github.io/Photo3/. It was created by Samantha Hartzell, Mark Bartlett, and Amilcare Porporato (email aporpora@princeton.edu, phone 609 258 2287), and first made available in 2017. Photo3 was developed in Python 2.7 with the SciPy, NumPy, Pandas, Tkinter, and Matplotlib packages. Program size is 45.6 kB. We suggest installing a Python distribution such as Anaconda to meet the program requirements.

Acknowledgements

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Appendix A. Details of the general photosynthetic model

The Rubisco-limited rate of carbon assimilation, $A_{oci}$, is given by

$$A_{oci}(c_{i}, T) = V_{c, max} \frac{c_{i} - \Gamma^{*}(T)}{c_{i} + K_{c}(T)/(1 + s_{i}/K_{c}(T))},$$

where $V_{c, max}$ is the maximum carboxylation rate, $c_{i}$ is the relevant CO2 concentration (see Eq. (4)), $K_{c}(T)$ and $s_{i}$ are the Michaelis-Menten coefficients for CO2 and O2, respectively, $c_{i}$ is the oxygen concentration, and $\Gamma^{*}$ is the CO2 compensation point (see Table 1 for the model parameters). The maximum carboxylation rate, $V_{c, max}$, and the CO2 compensation point, $\Gamma^{*}$, are given by

$$V_{c, max}(T) = V_{c, max0} \frac{\exp[H_{o2}/RT][1 - T_{o2}/T]}{1 + \exp(S_{c}[T - H_{o2}/RT])},$$

and

$$\Gamma^{*}(T) = \Gamma_{0}[1 + \Gamma_{1}(T - T_{0}) + \Gamma_{2}(T - T_{0})^{2}],$$

where $R$ is the universal gas constant (J/(mol K)), $T_{0}$ is a reference temperature, and the remaining parameters are given in Table 1. The temperature dependence of the Michaelis–Menten constants $K_{c}$ and $K_{c}$ is described by a modified Arrhenius equation, i.e.,

$$K_{c}(T) = K_{c0} \exp \left[ \frac{H_{c0}}{RT} \left( 1 - \frac{T_{c0}}{T} \right) \right].$$

The light-limited assimilation rate, $A_{co2}$, is given by
\[ A_s(\phi, c, T_l) = \frac{J(\phi, T_l) \left( c - \Gamma^s(T_l) \right)}{4 \left( c + 2\Gamma^s(T_l) \right)}. \]  

where \( J \), the electron transport rate, is equal to \( \min(J_{\text{max}}(T_l), J_\phi(\phi)) \). The maximum potential electron transport rate, \( J_{\text{max}}(T_l) \), is given by

\[ J_{\text{max}}(T_l) = J_{\text{max0}} \frac{\exp[H_s/RT_l(1 - T_d/T_l)]}{1 + \exp(S_{\text{air}} T_l - H_s/RT_l)}. \]

while the PAR limited electron transport rate, \( J_\phi(\phi) \), is given by

\[ J_\phi = \frac{\phi l^2}{2N_\phi h c}. \]

where \( \phi \) is the incoming radiation (W/m²), 50 percent of which is considered photosynthetically active radiation (PAR) (Jones, 1992), \( \lambda \) is the average wavelength (m) for PAR (assumed to be 550 nm), \( h \) is Planck’s constant (Js), \( c \) is the speed of light (m/s), \( N_\phi \) is Avogadro’s constant (mol⁻¹), and \( l^2 \) is the quantum yield of photosynthesis in mol CO₂ mol⁻¹ photons.

The dark respiration \( R_d \) is modelled according to an identical Arrhenius equation with coefficients \( R_{a0} \) and \( H_{aR} \) (see Leuning, 1995; Bartlett et al., 2014).

Appendix B. Details of the hydraulic model

Water potentials

The soil water potential, \( \psi_s \), is related to the soil moisture through a strongly nonlinear function given by Rodriguez-Iturbe and Porporato (2004) and Daly et al. (2004) as

\[ \psi_s(w) = \psi_s^* s^{-b}, \]

where \( \psi^*_s \) is the soil water potential at saturation and \( b \) is the exponent of the retention curve. The specific plant water capacitance \( c \), is defined as the change in relative stored water volume per unit change in water potential \( (c = dw/d\psi_s) \). In this study we have chosen to approximate the plant water capacitance as constant and the stored water potential \( \psi_w \) as a linear function of the relative water storage volume \( w \) following Hunt et al. (1991), i.e.,

\[ \psi_w(w) = \frac{w - 1}{c}. \]

This relationship neglects nonlinearities in the pressure-volume relationship caused by osmotic effects at low \( w \) in order to include plant water storage with a minimum level of complexity. Although a simplification, this linear relationship is a good approximation in the physically relevant regime for many succulent and CAM species (Nobel and Jordan, 1983; Hunt and Nobel, 1987; Ogburn and Edwards, 2012). In O. ficus-indica specifically, the pressure-volume relationship has been shown to be approximately linear for relative water contents above 20%; below this point further decreases in relative water content will lead to tissue damage and are not considered reversible (Goldstein et al., 1991).

(B.3) Conductances

The stomatal conductance to water, \( g_{s_{H2O}} \), is closely related to the stomatal conductance for CO₂ given in Eq. (2) and is here given by

\[ g_{s_{H2O}} = 1.6g_{s_{CO2}} + g_{s_{cut}}, \]

where the factor 1.6 accounts for the differences between the diffusivity in air of CO₂ and H₂O (Jones, 1992). The cuticular conductance, \( g_{s_{cut}} \), is added to the stomatal conductance to account for the small amount of water vapor lost in the absence of carbon assimilation (Burghardt and Riederer, 2003).

Following Daly et al. (2004), the soil-root conductance, \( g_w \), is assumed to be proportional to the soil hydraulic conductivity, \( K(s) \), divided by the average distance from the soil to root surface, i.e.,

\[ g_w(s) = \frac{K(s)\sqrt{RA_l s^{-d}}}{\pi g_\rho Z r}, \]

where \( R_A_l \) is the root area index under well-watered conditions, \( s^{-d} \) is a term introduced to model root growth under water-stressed conditions, \( g \) is the gravitational constant, and \( Z_r \) is the rooting depth. The hydraulic conductivity \( K(s) \) is given by

\[ K(s) = K_s s^{b+1}, \]

where \( K_s \) is the saturated hydraulic conductivity and \( b \) is a parameter defined in Eq. (B.1) (see Table 5).

The decrease in plant conductance under water stress is modeled by a vulnerability curve so that \( g_w \) is close to \( g_{w_{max}} \) for high \( \psi_w \) and is close to 0 for low \( \psi_w \) due to xylem cavititation (Sperry et al., 1998; Daly et al., 2004), i.e.,

\[ g_w = g_{w_{max}} \exp \left[ -\left( \frac{\psi_w}{j} \right)^h \right]. \]

where \( h \) and \( j \) are shape parameters. Following Waring and Running (1978) and Carlson and Lynn (1991), the conductance between the water storage tissue and the xylem is assumed to decrease with the fraction of stored water following a power law given by

\[ g_w = g_{w_{max}}^\mu w^\nu, \]
where \(g_{w,\text{max}}\) is the maximum storage-xylem conductance and \(a\) is a parameter between 1 and 10, here assumed to be equal to 4. Due to the linear relationship between \(w\) and \(\psi_x\), imposed by Eq. (B.2), this assumption is equivalent to assuming a power law relationship between the stored water potential \(\psi_x\) and the conductance \(g_w\).

### (B.8) Hydrology balance with plant water storage

In the absence of plant water storage, the hydrology balance may be described through Eqs. (13)–(15), which are solved simultaneously for the leaf water potential, \(\psi\), the leaf temperature, \(T_l\), and the transpiration \(E\). When plant water storage is included, the formulation of hydrology balance is slightly altered, and a fourth variable, \(\psi_x\), is introduced, which describes the water potential at the storage connection node. Eq. (14) is now given by

\[
E = \frac{g_w}{1 - f} (\psi_x - \psi),
\]

(B.8)

where \(g_w/1 - f\) is the hydraulic conductance between the storage connection node and the leaf (see Fig. 3). Now the hydraulic balance is described by Eqs. (13), (15), (17), and (B.8). To solve this system of equations, Eq. (B.8) is solved for \(\psi_x\) and substituted into Eq. (17), eliminating the unknown \(\psi_x\), i.e.

\[
E = \left( \frac{g_w}{1 - f} \right) \psi_x + \frac{1}{1 - f} \frac{\text{LA} g_p (\psi_x - \psi)}{g_w} + \frac{1}{1 - f} \frac{\text{LA} g_p (\psi_x - \psi)}{g_w},
\]

(B.9)

The resulting system of three equations – Eq. (13), (15), and (B.9) – is now solved simultaneously for the three unknowns, \(\psi_x\), \(T_l\), and \(E\).

### Appendix C. Details of the CAM photosynthetic model

The CAM photosynthetic fluxes \(A_{w}, A_{u}, A_{vc}\) are modified from Bartlett et al. (2014) to improve model robustness to a range of environmental conditions. The flux \(A_{vc}\) from the stomata to the Calvin cycle is given by

\[
A_{vc}(\phi, c_{m}, T_l, \psi_x, T, M) = \max \left\{ \phi \left[ \frac{A_{\phi \psi_{\text{nt}}} (\phi, c_{m}, T_l) - R_{\phi} (T_l)}{f_x (\psi)} \right] \left( 1 - f_C \left[ z, M \right] \right) \right\}.
\]

(C.1)

where \(R_{\phi}(T_l)\) is the respiration flux to the Calvin cycle and is given by

\[
R_{\phi}(T_l) = R_{\phi}(T_l) (1 - \exp(\phi)).
\]

(C.2)

The carbon function \(f_C(z, M)\) accounts for the circadian rhythm control of the flux dictated by the values of \(M\) and \(z\) and is given by

\[
f_C(z, M) = \left( 1 - f_{f}(z) \right) \frac{M}{\mu M_{\text{max}} + M}\]

(C.3)

where the order function \(f_{f}(z)\) describes the relative rate of malic acid diffusion from the cell vacuole to the cytoplasm and the overall activation state of the decarboxylation enzymes and is given by

\[
f_{f}(z) = \exp \left( - \left( \frac{z}{\mu} \right)^{c_{3}} \right),
\]

(C.4)

where \(\mu\) and \(c_{3}\) are circadian oscillator constants given in Table 2. Note that for \(f_{f} = 0\) the flux \(A_{vc}\) is the same as the C3 carbon assimilation given in Eq. (3).

The flux \(A_{w}\) from the stomata to the vacuole is adjusted from Bartlett et al. (2014) with a modification which prevents the flux from occurring when light is present and the vacuole is empty. The modified flux is given by

\[
A_{w}(T_l, \psi_x, T, z, M) = \left\{ \begin{array}{ll}
0, & \phi > 0 \text{ and } M < 1 \\
\left( A_{\phi \psi_{\text{nt}}} (T_l) - R_{\phi} (T_l) \right) f_x (\psi), & \text{otherwise},
\end{array} \right.
\]

(C.5)

where the malic acid storage function \(f_{\text{M}}(z, M, T_l)\) accounts for the circadian control of the flux and is given by

\[
f_{\text{M}}(z, M, T_l) = f_{f}(z) \frac{M_{\text{M}}(T_l) - M}{\mu M_{\text{M}}(T_l) + (M_{\text{M}}(T_l) - M)},
\]

(C.6)

where \(M_{\text{M}}(T_l)\) is the maximum storage concentration of malic acid and is given by

\[
M_{\text{M}}(T_l) = \mu M_{\text{max}} \left\{ \frac{T_{hi} - T_l}{T_{hi} - T_{lo}} (1 - \alpha_{2}) + \alpha_{2} \right\},
\]

(C.7)

where \(T_{hi}\) and \(T_{lo}\) are the high and low temperature bounds of the circadian rhythm and \(a_2\) is a parameter of the circadian oscillator. \(R_{\phi}(T_l)\) is the respiration flux to the cell vacuole, given by

\[
R_{\phi}(T_l) = R_{\phi}(T_l) \exp(-\phi).
\]

(C.8)

Finally, the flux \(A_{vc}\) from the vacuole to the Calvin cycle is given by

\[
A_{vc}(\phi, c_{v}, T, z, M) = \left( A_{\phi \psi_{\text{nt}}} (T_l) - R_{\phi} (T_l) \right) f_C(z, M).
\]

(C.9)
References


Bremner, P., Preston, G., Fazekas, C., de St, C.G., 1986. A


