Simulating daily field crop canopy photosynthesis: an integrated software package

Short running title: Diurnal canopy photosynthesis simulator (DCaPS)

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Summary Text

In the near future, global demand for agricultural product is predicted to surpass our production capacity and enhancing plant photosynthesis may be a solution for crop yield improvement. To accelerate enhancement, we need to know which target(s) should be manipulated for greatest impact, therefore, a modelling tool is developed. The tool will be able to improve our understanding of photosynthetic manipulation impacts on crop biomass accumulation, which ultimately affects crop yield.

Abstract

Photosynthetic manipulation is seen as a promising avenue for advancing field crop productivity. However, progress is constrained by the lack of connection between leaf-level photosynthetic manipulation and crop performance. Here we develop a model of diurnal canopy photosynthesis for well-watered conditions by using biochemical models of C₃ and C₄ photosynthesis upscaled to the canopy level using the simple and robust sun-shade leaves representation of the canopy. The canopy model was integrated over the time course of the day for diurnal canopy photosynthesis simulation. Rationality analysis of the model showed that it simulated the expected responses in diurnal canopy photosynthesis and daily biomass accumulation to key environmental factors (i.e. radiation, temperature and CO₂), canopy attributes (e.g. leaf area index and leaf angle) and canopy nitrogen status (i.e. specific leaf nitrogen and its profile through the canopy). This Diurnal Canopy Photosynthesis Simulator (DCaPS) was developed into a web-based application (www.dcaps.net.au) to enhance usability of the model. Applications of the DCaPS package for assessing likely canopy-level consequences of changes in photosynthetic properties and its implications for connecting photosynthesis with crop growth and development modelling are discussed.

Key words

Canopy photosynthesis, CO₂ partial pressure, Temperature effects, Dry matter accumulation, Radiation, Modelling

Introduction

The next advance in field crop productivity will likely need to come from improving crop use efficiency of resources (e.g. radiation, CO₂, water and nitrogen), aspects of which are closely
linked with overall crop photosynthetic efficiency (Long et al. 2015). For this, there is an emerging agenda focused on genetic manipulation of the biochemical pathway of photosynthesis aiming to enhance photosynthesis for improved crop yield (Evans 2013; Long et al. 2015). However, progress is limited by the lack of connection between biochemical/leaf-level photosynthetic manipulation and crop performance, which is influenced by interactions between (photosynthetic) genetic controls, plant growth and development processes, and environmental effects. Crop models that can incorporate the interactions and integrate across scales of biological organisation might be the tool needed to accelerate progress in photosynthetic enhancement (Wu et al. 2016).

In many crop models, used for seasonal simulation of crop growth, development and yield, daily biomass accumulation, which is determined by canopy photosynthesis, is a key driver of crop growth that has been used to simulate source-limited plant growth. Canopy photosynthesis modelling began with empirical models of leaf photosynthetic light response (PLR), which were upcaled and integrated to simulate diurnal canopy photosynthesis (Monsi and Saeki 1953; Hammer et al. 2009). There are multiple approaches for such upscaling, which focused on modelling the heterogeneous light environment within the canopy. These can be classified into models with “simplified” canopy representation, such as multi-layer models (each layer partitioned into sunlit and shade leaf fractions) (Duncan et al. 1967), single-layer big-leaf models (Sellers et al. 1992; Sands 1995) or (single-layer) sun-shade leaves models (Hammer and Wright 1994; de Pury and Farquhar 1997). Another type of approach is detailed models, such as static 3D and dynamic 3D (Vos et al. 2010) canopy architecture models. The respective (dis)advantages of these models have been discussed (Wu et al. 2016) and many have supported the simplicity and robustness of the sun-shade leaves approach. This approach can use either single or multiple layers with canopy leaf area index in each layer(s) partitioned into sunlit and shade leaf fractions. Another widely used type of canopy photosynthesis simulation, which avoids the need for photosynthesis modelling and upscaling, is to utilise a simple empirical linear relationship between crop (above-ground) biomass accumulation and intercepted solar radiation (or Radiation Use Efficiency, RUE) (Sinclair and Muchow 1999). Theoretical derivations have shown consistencies between the PLR and RUE approaches to modelling (Hammer and Wright 1994). Both types underpin source-limited plant growth simulation, which can be connected with crop models that incorporate both source- and sink-limited crop growth (Hammer et al. 2010). For example, the APSIM crop models (Hammer et al. 2009) provide important effects
that can regulate canopy photosynthesis via crop nitrogen status, which influences photosynthetic capacity. This is an effective and robust framework for connecting photosynthesis with crop growth, development and yield simulation (Wu et al. 2016).

Given the focus of photosynthetic enhancement at the biochemical level for field crop improvement, the PLR and RUE types of canopy photosynthesis modelling may not be adequate despite their apparent success in crop models. Their responses to variations at the biochemical level and to environment are difficult to predict due to the aggregated nature of the models. To overcome the limitations, canopy models based on more mechanistic photosynthesis models [e.g. C₃ and C₄ photosynthesis models; von Caemmerer (2000)] have emerged (de Pury and Farquhar 1997) and have been incorporated into vegetation growth models [e.g. BioCro: biocro.r-forge.r-project.org; Ecosys: ecosys.ualberta.ca; GECROS: Yin and van Laar (2005); WIMOVAC: Humphries and Long (1995)]. Most of them have utilised the simple and robust sun-shade leaves approach. However, there are only a limited number of such canopy photosynthesis models being applied in crop models (Yin and Struik 2008). Despite a limited number, these examples of modelling work demonstrated the value of using biochemical based canopy photosynthesis models to expand the biological functionality of crop models, which could potentially aid progress in photosynthetic enhancement for field crop improvement.

Besides the eventual target of incorporating diurnal canopy photosynthesis into field crop performance prediction, there is also a need for developing a standalone diurnal canopy photosynthesis simulator. This is likely to stimulate and guide different approaches to leaf-level photosynthesis research and reinforces thinking at the canopy level. For example, correlating Rubisco carboxylation rate with leaf nitrogen content would be useful for simulation of instantaneous canopy photosynthetic rate (de Pury and Farquhar 1997). More examples of relationships between photosynthetic and plant attributes have also emerged (Braune et al. 2009). As discussed above, there are existing examples of canopy models, however they have been developed as integrated modules in more extensive vegetation growth models. A standalone diurnal canopy photosynthesis simulator that informs canopy CO₂ assimilation/biomass accumulation in terms of photosynthetic attributes and diurnal environment would be a desirable tool. Such a tool can be utilised to aid the wider community of photosynthesis experimentalists to understand consequences at a higher level over a longer simulation period, as well as providing a valuable teaching tool.
The rationale of extending crop modelling and aiding progress in photosynthesis research warrant the development for a standalone tool of diurnal canopy photosynthesis simulation. It will need to incorporate the biochemical models of photosynthesis as well as respond to diurnal environment effects for simulating canopy CO$_2$ assimilation/biomass accumulation of a field crop over a day. To develop such a tool, three objectives have been identified:

1. develop a standalone C$_3$ and C$_4$ diurnal canopy photosynthesis simulator (DCaPS) for both C$_3$ and C$_4$ photosynthesis based on the concept of a cross-scale modelling framework that facilitates connection with crop growth and development dynamics (Wu et al. 2016)

2. present model rationality tests by simulating responses to key environmental factors (i.e. light, CO$_2$ and temperature), canopy nitrogen status (i.e. specific leaf nitrogen and its profile through the canopy), and canopy attributes and architecture (i.e canopy leaf area index and leaf angle);

3. develop DCaPS into an interactive web-based application that can be accessed using internet browsers on any major platform for simulating likely canopy-level consequences of photosynthetic changes.

The implications of the DCaPS package for crop modelling and its applications for photosynthetic manipulation are also discussed.

**Model overview**

The Diurnal Canopy Photosynthesis Simulator (DCaPS) calculates diurnal (period from sunrise to sunset) canopy CO$_2$ assimilation and daily (24h) biomass increment for a crop under well-watered conditions. A schematic diagram of the model is provided in Figure 1, model detail in the next section, and a comprehensive description and list of model equations and parameters in Tables 1, 2 and the appendices. Daily values of incident solar radiation, air temperature ($T_a$) and air vapour pressure deficit ($VPD_a$), commonly used in crop models, were used to derive instantaneous values at the start of each hour over the diurnal period. A single-layer sunlit and shade leaf modelling approach was used. Canopy leaf area index ($LAI_{can}$) was partitioned into sunlit and shade leaf fractions using the sun-shade leaves modelling approach (Hammer and Wright 1994; de Pury and Farquhar 1997) to calculate the amount of PAR absorbed by each fraction. $T_a$ was assumed as a proxy for leaf temperature ($T_l$), which affects photosynthetic physiology. The canopy profile of leaf nitrogen on a leaf area basis (specific
leaf nitrogen, SLN) was input and used to calculate the maximum rate of Rubisco
carboxylation (V\text{cmax}), the maximum rate of electron transport (J\text{max}) and the maximum
phosphoenolpyruvate (PEP) carboxylase activity (V\text{pmax}) (de Pury and Farquhar 1997), which
are parameters of the C\text{3} and C\text{4} photosynthesis models (Farquhar \textit{et al.} 1980; von Caemmerer
2000) used in DCaPS. The photosynthesis models were coupled with a CO\text{2} diffusion model
to calculate C\text{c} and CO\text{2} assimilation rate. Photosynthesis of both the sunlit and shade leaf
fractions of the canopy were calculated, summed for the canopy, integrated hourly, and
summed over the diurnal period to calculate total diurnal canopy photosynthesis, which was
taken as the daily sum. This was converted to daily total biomass increment (BIO\text{total,\text{DAY}})
amsuming a conversion ratio (B), which combines factors allowing for biochemical
conversion and maintenance respiration (Sinclair and Horie 1989). A fraction of BIO\text{total,\text{DAY}}
was partitioned to root and the remaining amount was taken as the daily above-ground
canopy (shoot) biomass increment (BIO\text{shoot,\text{DAY}}).

\textbf{Model detail}

\textit{Absorbed photosynthetic active radiation (PAR)}

In both the C\text{3} and C\text{4} photosynthesis models (not replicated here, but detailed in Appendix A),
the potential electron transport rates (J, \text{\mu}mol \text{\ e}^{-}\text{\ m}^{-2}\text{\ s}^{-1}) of sunlit and shade leaf fractions are
driven by absorbed photosynthetic active radiation (PAR) using a non-rectangular hyperbolic
function (von Caemmerer 2000). Absorbed PAR for each of the sunlit and shade leaf fractions
varies diurnally and its calculation requires diurnal total incident solar radiation, LAI\text{can}, canopy
architecture (in the form of canopy-average leaf angle), and optical properties (reflectance and
transmittance) of leaves. Separation of absorbed PAR for the sunlit and shade leaf fractions of
the canopy is a necessary detail to avoid errors in over estimation of photosynthetic rate (de
Pury and Farquhar 1997).

The calculation of diurnal absorbed PAR depends on the radiation environment (Hammer and
Wright 1994). Firstly, diurnal extra-terrestrial radiation (S\text{0}, \text{MJ} \text{\ m}^{-2}\text{\ ground day}^{-1}) was
calculated from latitude (\text{Lat}, radians) and day of year (DAY) (Eqn A5). Then diurnal total
incident solar radiation on the ground (S\text{g}, \text{MJ} \text{\ m}^{-2}\text{\ ground s}^{-1}) was calculated by multiplying S\text{0}
and the atmospheric transmission ratio (RATIO) (Eqn A4). S\text{g} was then distributed sinusoidally
over the diurnal period to derive instantaneous values for incident radiation (I\text{0} \text{MJ} \text{\ m}^{-2}\text{\ ground

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(Eqn A3). \( I_\circ \) consists of direct (\( I_{\text{dir}} \), MJ m\(^{-2}\) ground s\(^{-1}\)) and diffuse (\( I_{\text{dif}} \), MJ m\(^{-2}\) ground s\(^{-1}\)) radiation components. Diffuse radiation represents 17% of solar insolation (\( S_0 \)) for any \( \text{Lat}, \ \text{DAY} \) and \( \text{RATIO} \) (Eqn A1). The diurnal pattern of atmospheric transmission of \( I_{\text{dir}} \) is more complex, so was simply obtained by the difference between \( I_\circ \) and \( I_{\text{dif}} \) (Eqn A2). This approach allows the proportion of \( I_{\text{dir}} \) and \( I_{\text{dif}} \) to vary across a diurnal period giving, for example, higher proportion of \( I_{\text{dif}} \) in early and later hours of the diurnal period and higher proportion of \( I_{\text{dif}} \) if \( \text{RATIO} \) is low due to cloud cover.

The derived \( I_{\text{dir}} \) and \( I_{\text{dif}} \) (total incident solar radiation) from above were used to estimate direct and diffuse PAR (\( I_{\text{dir,PAR}} \) and \( I_{\text{dif,PAR}} \), respectively). It was assumed that 50% of the energy in \( I_{\text{dir}} \) and \( I_{\text{dif}} \) was PAR, which was converted to photosynthetic photon flux density by multiplying by 4.56 and 4.25 μmol PAR (J PAR\(^{-1}\))\(^{1}\), respectively (Eqns A21 and A22). Units for \( I_{\text{dir,PAR}} \) and \( I_{\text{dif,PAR}} \) are μmol PAR m\(^{-2}\) ground s\(^{-1}\).

The PAR absorbed by either sunlit or shade leaves fractions (\( I_{\text{abs,sun}} \) and \( I_{\text{abs,sh}} \), both with units of μmol PAR m\(^{-2}\) s\(^{-1}\)) was calculated using the equations of de Pury and Farquhar (1997). This incorporated \( I_{\text{dir,PAR}} \) and \( I_{\text{dif,PAR}} \), optical properties of leaves, such as reflectance and transmittance to PAR, LAI\(_{\text{can}}\), and the proportion of intercepted radiation (dependent on canopy-average leaf angle and LAI\(_{\text{can}}\)). It was assumed that the sunlit leaf fraction received \( I_{\text{dir,PAR}} \), \( I_{\text{dif,PAR}} \) and scattered radiation (caused by reflectance and transmittance of leaves), while the shade leaf fraction received only \( I_{\text{dif,PAR}} \) and scattered radiation. Detailed equations and calculation procedures are given by Eqns A19–A32 in Appendix A. In the current model, diurnal variations in leaf reflectance and transmittance are not considered. However, as a first approximation, it can be input into DCaPS for each diurnal simulation.

**Air vapour pressure deficit (\( \text{VPD}_a \))**

Air vapour pressure deficit (\( \text{VPD}_a \), kPa) was calculated as the difference between the saturated vapour pressure at air temperature (\( \text{SVP}_a \)) and that at dew-point temperature (\( \text{SVP}_d \)) (Eqns A16–A18). The minimum temperature (\( T_{a,\text{min}} \); more below) for the day was assumed as the dew-point temperature, which has been shown to give robust estimates of \( \text{VPD}_a \) (Lobell *et al.* 2015). Accordingly, \( \text{VPD}_a \) varies diurnally with air temperature.
Specific leaf nitrogen (SLN) and photosynthetic physiology

Specific leaf nitrogen (SLN, g N m$^{-2}$ leaf) influences key photosynthetic physiological parameters. Using the mathematical development by de Pury and Farquhar (1997), vertical variation through the canopy can be explicitly incorporated; the approach integrates the profile to give a total for the single-layer canopy, which is then partitioned into sunlit and shade leaves. Distribution of SLN in the canopy was assumed to follow an exponential decay with canopy depth (Eqn A34). The decay function was specified by SLN at the top layer of the canopy ($SLN_o$, g N m$^{-2}$ leaf) and the average SLN for the canopy ($SLN_{av}$, g N m$^{-2}$ leaf). To incorporate the effects of SLN on photosynthetic physiology, this model assumed that at the reference temperature of 25°C, the maximum rate of Rubisco carboxylation ($V_{cmax}$), the maximum rate of electron transport ($J_{max}$), leaf day respiration ($R_d$), and the maximum PEP carboxylase activity ($V_{pmax}$) were all zero below a minimum SLN and increased linearly with slope of $\chi_V$, $\chi_R$ and $\chi_P$, respectively, above that threshold value (Eqns A37–A40). The minimum SLN values were 0.35 and 0.2 g N m$^{-2}$ (leaf) for C$_3$ and C$_4$, respectively (Table 1).

Leaf temperature ($T_l$)

Estimation of air temperature ($T_a$, °C) is needed as it significantly influences leaf temperature ($T_l$, °C). A model of daily $T_a$ (over the 24h) was used (Eqn A15). Even though the majority of daylight hours can be modelled by the diurnal function of the model, the night time function is sometimes applicable for the early hours of the diurnal period. The diurnal period was modelled with a sine function and an exponential decay function was used during the night. The amplitude of the daily $T_a$ fluctuation was specified by the maximum ($T_{a,max}$, °C) and minimum ($T_{a,min}$, °C) air temperature of the day. The phase shift of the sine function was determined by the lag coefficient for the maximum temperature ($x_{lag}$), the night-time temperature coefficient ($y_{lag}$), and the lag of minimum temperature from the time of sunrise ($z_{lag}$) (Eqn A15). It was assumed here that $T_l$ is approximated by $T_a$ for both sunlit and shade leaf fractions. This is a reasonable assumption over a wide range of temperature under well-watered conditions.

The response of photosynthesis to $T_l$ was modelled through responses of the C$_3$ and C$_4$ photosynthesis model parameters to $T_l$ (i.e. $K_c$, $K_v$, $V_{omax}/V_{cmax}$, $V_{cmax}$, $J_{max}$ and $R_d$ for C$_3$ plus $K_p$ and $V_{pmax}$ for C$_4$; Table 1). There is a growing availability of these temperature responses, in particular, for model species. The most comprehensive data set for the C$_3$ Nicotiana tabacum have been used effectively for simulating temperature responses of leaf
photosynthesis (Bernacchi et al. 2002). Temperature responses of $K_c$, $K_o$ and $V_{\text{omax}}/V_{\text{cmax}}$ are usually assumed to be similar among C$_3$ species (von Caemmerer 2013), so here we used parameters from *Nicotiana tabacum* for C$_3$ crop species. It was reported that $K_c$ of *Triticum aestivum* is significantly different to *Nicotiana tabacum* (Sharwood et al. 2016), but whether or not this has significant implications for diurnal canopy photosynthesis will require sensitivity analysis when other wheat parameters also become available. Parameter availability for C$_4$ crop species is not as comprehensive so here we used parameters for the C$_4$ model species *Setaria viridis* (Boyd et al. 2015). These default values can be readily changed as parameters of C$_4$ crop species become better known.

Temperature responses of $K_c$, $K_o$, $V_{\text{cmax}}$, $R_d$, $K_p$ and $V_{\text{pmax}}$ were modelled using an exponential type function [Eqn 1, adapted from Sharkey et al. (2007)], whereas $J_{\text{max}}$, due to its apparent optimum in temperature response (Farquhar et al. 1980), was modelled via a normal distribution function [Eqn 2, adapted from June et al. (2004)]. $V_{\text{cmax}}/V_{\text{omax}}$ and its temperature response were not available from Bernacchi et al. (2002), where $K_c$ and $K_o$ were reported, but can be back calculated from $K_c$, $K_o$ and $T^*$ with Eqns A52 and A53 (assuming a chloroplastic oxygen partial pressure ($O_c$) of 210000 μbar). Its temperature response can be modelled with Eqn 1. In summary, temperature responses of the C$_3$ and C$_4$ photosynthesis model parameters to $T_l$ were modelled with Eqn 1 or 2 with parameter values given in Table 2.

Expression of the exponential type function used to describe temperature response of certain photosynthesis model parameters [adapted from Sharkey et al. (2007)]:

$$P = P_{25} e^{(c-b/(T_l+273))}$$

(Eqn 1)

where $P_{25}$ is the modelled value of parameter at 25°C, $c$ and $b$ are empirical constants, which are balanced to give the factor after $P_{25}$ unity at 25°C. Expression of the normal distribution function [adapted from June et al. (2004)]:

$$P = P_{25} e^{((-T_l-T_{\text{opt}})/\theta)^2 + (25-T_{\text{opt}}/\theta)^2}$$

(Eqn 2)

where $T_{\text{opt}}$ is the optimum temperature and $\theta$ is the difference in temperature from $T_{\text{opt}}$ at which $P$ falls to $e^{-1}$ (0.37).

**Chloroplastic CO$_2$ partial pressure ($C_c$)**

Air CO$_2$ ($C_a$, μbar) has to diffuse into leaves to reach the carboxylating site of Rubisco inside the chloroplasts for photosynthesis. The best practice for expressing CO$_2$ levels is in partial
pressure (Sharkey et al. 2007). To convert from the usual unit of ppm to μbar, it was
multiplied by the air pressure (e.g., at sea level, CO$_2$ of 400 ppm is (400×10$^{-6}$)×
1013250 μbar = 405.3 μbar). Leaf boundary-layer and stomatal conductance have
significant effects on the drawdown of intercellular airspace CO$_2$ partial pressure ($C_i$) relative
to $C_a$ (Leuning 1995) and mesophyll conductance has significant effects on the drawdown of
CO$_2$ partial pressure at the carboxylating site of Rubisco ($C_c$) relative to $C_i$ (Flexas et al.
2012). Diffusional conductance, the reciprocal of resistance, of these three components [i.e.
leaf boundary-layer ($g_{lb}$), stomatal ($g_s$) and mesophyll ($g_m$) conductance] are incorporated in
$C_c$ estimation (Eqn A47) based on Fick’s first law of diffusion. To model crop canopies, the
turbulent resistance through the canopy boundary layer, which would affect CO$_2$ partial
pressure, air temperature and vapour pressure deficit (relative to those above the canopy),
needs to be considered (Leuning et al. 1995). However, in their modelling work, Leuning et
al. (1995) showed simulated canopy photosynthesis reproduced features in data so the
omission of the turbulent resistance is a reasonable approximation.

However, there are uncertainties in the estimation of $g_{lb}$ and $g_s$. The model that is commonly
used for $g_{lb}$ estimation relies on leaf width and local wind speed (Goudriaan and van Laar
1994), which cannot be assigned a priori. Numerous types of leaf stomatal conductance ($g_s$)
models have been developed over the years (Damour et al. 2010). Two particular types are
widely used. These are the empirical multiplicative models of environmental influences such
as light, $C_a$ and VPD$_a$ [e.g. the Jarvis model; Jarvis (1976)] and the semi-empirical models
relating $g_s$ to photosynthesis with VPD$_a$ [e.g. the BWB model (abbreviated using authors’
names); Ball et al. (1987)], while more mechanistic models with plant physiology
considerations based on abscisic acid or hydraulic control have also been developed (Damour
et al. 2010). The limitation of the multiplicative type models is the lack of interactions
between plant physiology and among the environmental factors; while the models relating $g_s$
to photosynthesis rely on empirical parameters, which cannot be assigned a priori. These
empirical coefficients can vary greatly between C$_3$ species (Li et al. 2012) and so cannot be
generalised for C$_3$ crop species, while the coefficients are rarely reported for C$_4$ crop species.
Given that there are limited data available to calibrate the empirical coefficients of the Jarvis
or the BWB models for C$_3$ and especially C$_4$ crop species, an alternative approach to estimate
$C_i$ is to use the ratio of $C_i/C_a$, which is based on stomatal optimization theory in that stomata
respond to maintain a constant $C_i$ under a given $C_a$ to maximize CO$_2$ assimilation. This ratio
(~0.7 for C$_3$ and ~0.4 for C$_4$) has been found to be stable with $C_a$ between 100 μbar and 400
μbar in combination with any PPFD between 250 μmol m$^{-2}$ s$^{-1}$ and 2000 μmol m$^{-2}$ s$^{-1}$ (Wong et al. 1979); further, $C_i/C_a$ does not appear to change under elevated $C_a$ (Ainsworth and Long 2005). The consistency in $C_i/C_a$ in a wide range of conditions makes it an efficient and robust modelling approach. It is not clear how $C_i/C_a$ would respond to PPFD lower than 250 μmol m$^{-2}$ s$^{-1}$, but such conditions only apply to the very early and late hours in a diurnal period, which amount to less than ca. 5% of diurnal canopy photosynthesis and so any changes under such conditions would have limited effect on diurnal total estimation. However, like $g_s$, $C_i/C_a$ is influenced by VPD$_a$. It was found to decrease linearly with VPD$_a$ in various species including C$_3$ Oryza sativa and C$_4$ Zea mays (Zhang and Nobel 1996). $C_i/C_a$ response to VPD$_a$ can be given by:

$$C_i/C_a = aVPD_a + b$$

Eqn 3

where $a$ and $b$ are empirical constants. For C$_3$ they are -0.12 and 0.90, respectively; for C$_4$, they are -0.19 and 0.84, respectively. At VPD$_a$ between 1 to 2 kPa, Eqn 3 gives ~0.7 and 0.5 for C$_3$ and C$_4$, respectively, which are similar to those reported by Wong et al. (1979). Here, we used the simpler $C_i/C_a$ ratio approach for $C_c$ estimation (Eqn A49), which avoided the need for $g_h$ and $g_s$.

The importance of mesophyll conductance ($g_m$) has been recognised only recently. $g_m$ in model C$_3$ species is known to vary with temperature and there is evidence that $g_m$ may also respond to the other key environmental factors (e.g. irradiance and CO$_2$), but this variation is not yet completely certain (Pons et al. 2009). So here we included only the effect of temperature and modelled this by using the normal distribution function (Eqn 2). At the reference temperature (i.e. 25°C) $g_m$ (per leaf area) in C$_3$ wheat is assumed to be 0.55 mol CO$_2$ m$^{-2}$ s$^{-1}$ bar$^{-1}$. No values for C$_4$ species have been reported, so the C$_3$ value was used as a default value.

Diurnal canopy photosynthesis, daily respiration, root and canopy biomass accumulation, and RUE

Diurnal canopy CO$_2$ assimilation, daily respiration and conversion losses, and allowance for root biomass were used to calculate daily above-ground canopy (shoot) biomass increment (BIO$_{shoot,DAY}$). This model assumes that photosynthesis during the diurnal period results in carbon assimilation for the entire day so we use the symbol $A_{can,DAY}$. $A_{can,DAY}$ was calculated by summing the CO2 assimilation of the sunlit ($A_{sun}$) and shaded ($A_{sh}$) leaf fractions of the canopy at the start of each hour over the diurnal period, integrated hourly and summed over...
the diurnal period (Eqn A73). Using the C$_3$ and C$_4$ photosynthesis models, leaf respiration during the diurnal period can be implicitly accounted for at the leaf level with the parameter $R_d$ (Eqns A51, A54, A55 and A59). However, this lacks consideration of respiration from other plant organs and during the night period. A common approach is to omit the leaf-level $R_d$ (by setting $\chi_R$ to zero) and consider respiration at the plant level on a daily basis, which can be accounted for within a conversion ratio ($B$) that combines factors allowing for biochemical conversion of CO$_2$ to biomass and CO$_2$ loss due to maintenance respiration (Sinclair and Horie 1989). This approach is consistent with the conservative respiration:photosynthesis ratio approach (Gifford 2003), by which plant respiration is taken as a fraction of total canopy photosynthesis. The conversion ratio, $B$, is 0.41 g biomass (g CO$_2$)$^{-1}$ for cereal crops such as rice and maize (Sinclair and Horie 1989). Therefore, daily whole-plant biomass increment (BIO$_{total,DAY}$) was calculated by multiplying $A_{can,DAY}$ with the molecular weight of CO$_2$ (= 44 g (mol CO$_2$)$^{-1}$) and $B$. To calculate shoot biomass increment (BIO$_{shoot,DAY}$), BIO$_{total,DAY}$ is multiplied by the fraction of above-ground (shoot) biomass to total biomass (shoot + root), denoted by $P_{shoot}$ (Eqn A74). In effect, this simulates partitioning of a fraction of BIO$_{total,DAY}$ to root. Here, $P_{shoot}$ is given a default of 1 assuming a mature canopy around flowering.

Radiation Use Efficiency for the day (RUE$_{DAY}$, g biomass MJ$^{-1}$) was then calculated by dividing BIO$_{shoot,DAY}$ by the total amount of intercepted solar radiation (Eqns A75 and A76, respectively).

### Model rationality analysis

#### Environmental parameters

Default environmental parameters were set for C$_3$ wheat (winter crop) and C$_4$ sorghum (summer crop), with a canopy leaf area index ($LAI_{can}$) = 6, growing in the southern hemisphere spring ($DAY = 298$) and summer ($DAY = 15$), respectively, at locations with $Lat = -35^\circ$ and $-27.5^\circ$, respectively. Clear sky with atmospheric transmission ratio ($RATIO$) of 0.75 was assumed unless otherwise stated. The average maximum and minimum air temperatures at these times of year were 21 and 7°C for $Lat = -35^\circ$ and 30 and 15°C for $Lat = -27.5^\circ$.

#### Diurnal canopy photosynthesis in relation to canopy architecture

Diurnal patterns of net C$_3$ and C$_4$ canopy photosynthesis for a range of canopy LAI ($LAI_{can}$) and canopy-average leaf inclination relative to the horizontal ($\beta$) were simulated as a qualitative
test of the Diurnal Canopy Photosynthesis Simulator (DCaPS). The C₄ simulations (Figure 2C and D) were consistent in the diurnal pattern and magnitude with those reported by Duncan et al. (1967) and Hammer et al. (2009), who found that the canopy with erect leaves (β = 80°) continued to increase canopy photosynthetic rate beyond LAIₕₐₜ = 4 at high LAIₕₐₜ (= 8) due to better light distribution throughout the canopy. There was ca. 40% increase in midday canopy photosynthetic rate at LAIₕₐₜ = 8 compared to LAIₕₐₜ = 4, which was comparable to that simulated by Duncan et al. (1967) and Hammer et al. (2009). In the canopy with less erect leaves (β = 40°), there was little increase in canopy photosynthetic rate with increase in LAIₕₐₜ beyond 4. In terms of the magnitude, the simulated canopy photosynthetic rate at LAIₕₐₜ = 4 (Figure 2C and D) was comparable to that observed in a similar size maize canopy (~70 μmol CO₂ m⁻² s⁻¹) by Grant et al. (1989). The simulation also indicated that for a canopy with low LAIₕₐₜ (= 2), less erect leaves (β = 40°) offered greater PAR absorption by both sunlit and shade leaf fractions consistent with greater radiation interception as found by Hammer et al. (2009). Even though the sunlit LAI (LAIₜₐₜ) can be reduced up to 30% with less erect leaves, its photosynthetic rate was not affected due to associated increase in absorbed PAR. For the case of the shade leaf fraction, the increase in both the absorbed PAR and shade LAI (LAIₘₐₜ) significantly increased shade leaf Aᵥₕₐₜ. These consequences for the two leaf fractions translate to a greater canopy photosynthesis with less erect leaves at low LAIₕₐₜ. The effects of leaf erectness were mostly analogous for the C₃ simulations (Figure 2A and B). However, the greater radiation interception offered by less erect leaves at low LAIₕₐₜ did not translate to greater canopy photosynthesis. Unlike C₄, reduction in LAIₜₐₜ significantly reduced the Rubisco-limited photosynthetic rate (Aᵥₙₜ) resulting in reduced photosynthetic rate in the sunlit leaf fraction. This more than offset the increase (because of increase in both the absorbed PAR and LAIₘₐₜ) in Aᵥₘₐₜ. So in the case of C₃, Rubisco limitation can reduce photosynthetic rate of small (low LAIₕₐₜ) canopies with less erect leaves.

Diurnal canopy photosynthesis in relation to CO₂ with varying temperature

A simulation of net C₃ and C₄ diurnal canopy photosynthesis (Aᵥₜₒₜ,DAY) for a range of air CO₂ partial pressures (Cₐ) and temperatures (Tₐ) was undertaken as a qualitative test. Based on various large-scale free-air CO₂ enrichment (FACE) studies, elevating Cₐ to 475–600 μbar (or an average of 540 μbar) increased C₃ Aᵥₜₒₜ,DAY by an average of 28% relative to Cₐ = 360 μbar (Ainsworth and Long 2005). This increase was reproduced when Tₐₘᵦᵢₜ and Tₐₘᵦₓ were set to 14 and 28°C, respectively, simulating hot days for winter wheat crops (Figure 3). Ainsworth
and Long (2005) noted that when the large-scale free-air CO$_2$ enrichment (FACE) studies were
categorised by temperature, the relative increase in light saturated photosynthesis was lower
(an average of 19%) at lower temperatures (< 25°C). Simulation results for average days with
$T_{a_{\text{min}}}$ and $T_{a_{\text{max}}}$ of 7 and 21°C, respectively, is consistent with this CO$_2$ response at lower
temperatures (Figure 3). Increase in $A_{\text{can,DAY}}$ can be as high as 50% at $C_a = 1000$ μbar. This
result is discussed further below in regards to daily radiation use efficiency. In the case of C$_4$
canopy photosynthesis, the response of net $A_{\text{can,DAY}}$ to $C_a$ and temperature was significantly
less, which is consistent with the finding that C$_4$ maize photosynthesis is not significantly
affected by elevated $C_a$ (Leakey et al. 2006). This simulation suggested that canopy
photosynthesis of C$_3$ crops can significantly benefit from elevated CO$_2$, while C$_4$ crops do not.

**RUE$_{\text{DAY}}$ in relation to CO$_2$ with varying temperature**

A simulation of C$_3$ and C$_4$ daily canopy Radiation Use Efficiency (RUE$_{\text{DAY}}$) for a range of air
CO$_2$ partial pressures ($C_a$) and air temperatures ($T_a$) was also undertaken as a qualitative test.
Elevated $C_a$ is known to increase the net photosynthetic rate of C$_3$ plants resulting in increased
biomass accumulation and RUE (Kimball et al. 2002) and there is also an enhanced effect on
RUE at higher $T_a$ (Reyenga et al. 1999). The general consensus is that RUE of C$_3$ crops
increases almost linearly from $C_a$ of 300 to 660 μbar, reaches ca. 30% increase at double the
ambient $C_a$ and plateaus at ca. 50% beyond $C_a$ of 1000 μbar (Lobell et al. 2015). O'Leary et al.
(2015) found a ca. 22% increase in wheat crop biomass in response to elevated $C_a$ from 365 to
550 μmol mol$^{-1}$. These known responses of C$_3$ RUE were reproduced with the model for winter
wheat crops experiencing average to hot temperatures (Figure 3). The response relative of
RUE$_{\text{DAY}}$ to $C_a$ and temperature reflect that of net $A_{\text{can,DAY}}$ because of the linear relationship
between RUE$_{\text{DAY}}$ and $A_{\text{can,DAY}}$ (Eqns A74 and A75). In the case of the C$_4$ canopy, elevated $C_a$
had only a small effect on the simulated RUE$_{\text{DAY}}$ (Figure 3), which was consistent with a lack
of response to $C_a$ observed in C$_4$ sorghum. This simulation suggested that elevated CO$_2$ can
significantly benefit canopy biomass accumulation of C$_3$ crops, but not C$_4$ crops.

**RUE$_{\text{DAY}}$ in relation to average temperature**

A simulation of C$_3$ and C$_4$ daily canopy Radiation Use Efficiency (RUE$_{\text{DAY}}$) for a range of
average air temperature was undertaken as a qualitative test. Air temperature ($T_a$) varies
diurnally between the daily maximum ($T_{a_{\text{max}}}$) and minimum ($T_{a_{\text{min}}}$) temperature and the
A diurnal pattern can be modelled with Eqn A15. A 15°C difference between $T_{a,\text{max}}$ and $T_{a,\text{min}}$ was assumed and a range of temperature used so that temperatures ranging from 0–35°C for C3 and 10–40°C for C4 were included. When plotted against average daily temperature the simulated $\text{RUE}_{\text{DAY}}$ was relatively insensitive between average temperatures of 14–23°C for C3 and 21–28°C for C4 (Figure 4). This is consistent with known insensitivities of crop biomass accumulation and RUE to temperatures around optimal values (Yan and Hunt 1999). These temperature ranges for C3 and C4 responses were associated with the response of leaf photosynthesis to temperature, which is also insensitive within a broad range [e.g. C3: rice and wheat (Nagai and Makino 2009); C4: various grasses (Ludlow 1981), maize (response curve was derived from picking a typical $C_i$ (e.g. 150 µbar) in $A/C_i$ curves measured at different temperature in Massad et al. (2007)]. Further, RUE under optimum growth conditions has been reported as 1.2–1.5 g MJ$^{-1}$ for wheat (Fischer et al. 2014) and 1.2-1.4 g MJ$^{-1}$ for dwarf sorghum (George-Jaeggli et al. 2013). The simulated maximum $\text{RUE}_{\text{DAY}}$ for C3 and C4 corresponded with these reported ranges (Figure 4).

The comparison here between C3 wheat and C4 dwarf sorghum RUE does not reveal differences in magnitude between C3 and C4 crops, where the latter is typically higher. RUE of some tall hybrid sorghum varieties (George-Jaeggli et al. 2013) and maize (Sinclair and Muchow 1999) was found to be as high as 1.6-1.8 g MJ$^{-1}$, or possibly even higher (2.0-2.2 g MJ$^{-1}$) during the rapid stem elongation and maximum biomass accumulation phase (Olson et al. 2012). The typical high C4 RUE could be ascribed to higher photosynthetic rate (Hammer et al. 2010) and/or differences in canopy architecture, which may affect diurnal canopy photosynthesis (Figure 2). These scenarios (and their combinations) can be simulated with the model. As a demonstration of this capability, we have assumed the first case by increasing the slope of the linear relationship between the maximum rate of Rubisco carboxylation ($\chi_{V_c}$), maximum rate of electron transport ($\chi_I$), maximum PEP carboxylase activity ($\chi_{VP}$) and specific leaf nitrogen; these gave greater $V_{c,\text{max}}$, $J_{\text{max}}$ and $V_{p,\text{max}}$, respectively, and simulated the typical high RUE in C4 crops (Figure 4).

**RUE$_{\text{DAY}}$ in relation to $SLN_{av}$ with varying direct:diffuse radiation**

A simulation of C3 and C4 $\text{RUE}_{\text{DAY}}$ for a range of canopy-average specific leaf nitrogen ($SLN_{av}$) with varying direct:diffuse radiation was undertaken as a qualitative test. Direct:diffuse radiation was varied by changing the atmospheric transmission ratio ($\text{RATIO}$) in a similar
manner to the simulation study of Hammer and Wright (1994). High values \( RATIO = 0.75 \) reflect clear sky with high transmission of direct radiation and a low fraction of diffuse radiation. Massignam (2003) found that RUE of the C\(_3\) crop sunflower responded asymptotically to \( SLN_{av} \) with RUE of \( ca. 1 \) and \( 1.5 \) g MJ\(^{-1}\) at \( SLN_{av} \) of \( 1.5 \) and \( 2 \) g N m\(^{-2}\), respectively. This was closely predicted by the model with clear sky conditions (Figure 5A). Muchow and Sinclair (1994) found that RUE of field-grown dwarf sorghum responded asymptotically to \( SLN_{av} \), but did not approach the asymptote because sorghum \( SLN_{av} \) maximised at \( 1.3 \) g N m\(^{-2}\) giving RUE of \( 1.26 \) g MJ\(^{-1}\). This was also closely predicted by the model with clear sky conditions (Figure 5B). The simulated RUE\(_{DAY}\) response of typical dwarf sorghum was not significantly different from that for wheat, but when the model was parameterised for the greater photosynthetic rate of the tall hybrid sorghums, the response was higher at all \( SLN_{av} \) (Figure 5B). These responses were comparable to that of maize crops (RUE of \( ca. 1.5 \) and \( 2 \) g MJ\(^{-1}\) at \( SLN_{av} \) of \( 1 \) and \( 2 \) g N m\(^{-2}\), respectively) (Massignam 2003). In general, direct radiation level was higher with higher \( RATIO \), while the absolute level of diffuse radiation was insensitive to \( RATIO \), leading to a greater fraction of diffuse at low \( RATIO \) (cloudy days). Simulated results of increasing diffuse radiation fraction on C\(_3\) species (Figure 5A) were consistent with Tubiello et al. (1997), who found a significant increase (~40\%) in wheat RUE when grown under high diffuse radiation conditions due to the fact that diffuse radiation penetrates deeper into the crop canopy and increases photosynthetic rate of the lower leaves. Hammer and Wright (1994) used a simpler canopy photosynthesis model to show that decreases in \( RATIO \) caused RUE to increase. This response of RUE\(_{DAY}\) to \( RATIO \) was reproduced (Figure 5). While both C\(_3\) and C\(_4\) types responded similarly to the increased fraction of diffuse radiation, the standard C\(_4\) types achieved higher RUE\(_{DAY}\) at much lower \( SLN_{av} \) as a result of their greater photosynthetic rate (Figure 5B). This is consistent with the comparison of responses reported by Sinclair and Horie (1989).

### Applications for photosynthesis manipulation – a tool for assessing consequences of photosynthetic changes

The Diurnal Canopy Photosynthesis Simulator (DCaPS) enables simulation of likely canopy-level consequences of photosynthetic manipulation and canopy structural attributes in C\(_3\) and C\(_4\) field crops. It integrates many non-linear responses of leaf photosynthesis to environment and processes involved in upscaling to the canopy level (see Model Detail).
Considerable effort has been invested to develop DCaPS into an interactive web-based application (www.dcaps.net.au), which can be run with internet browsers on any major platform without prior installation of DCaPS (DCaPS v1.0 source code is available at https://github.com/QAAFI/DCaPS.git). This web-based application is conveniently available for experimentalists working on photosynthetic research and/or as a teaching tool. DCaPS can be parameterised for a range of environments, canopy attributes, and photosynthetic physiology. The online application reports diurnal patterns of environmental variables, diurnal canopy photosynthesis and daily canopy biomass increment.

Here we present two examples of using DCaPS to simulate consequences of changing photosynthetic attributes in both C3 and C4. These are simplified examples to demonstrate the capacity of DCaPS to capture complex dynamic interactions between photosynthetic physiology and diurnal variations in environment, which are not mechanistically included in, for example, the RUE type of canopy photosynthesis models. Users need to be aware of possible concomitant changes associated with changing model parameters. However, knowledge generated from exercising this model could inform photosynthetic manipulation efforts for assisting field crop improvement.

**Relative CO₂/O₂ specificity of Rubisco**

Increasing the relative CO₂/O₂ specificity of Rubisco (S_c/o) is a strategy for increasing CO₂ assimilation in isolated leaves (Evans 2013). There are likely concomitant changes associated with changing S_c/o (Evans 2013). However, in this simulation, we have minimised complexity by assuming all other parameters are kept at default values (Table 1 and 2).

Using DCaPS, it was estimated that a significant (25%) increase in S_c/o, could increase C3 and C4 diurnal canopy photosynthetic rate (A_can,DAY) by ca. 6.0% and 2.5%, respectively, assuming all other parameters were kept at default values (Tables 1 and 2). While S_c/o was set to increase by 25%, much of the enhancement was not translated to increase in photosynthetic rate as Rubisco-limited photosynthesis is less sensitive to changes in S_c/o than electron transport limited photosynthesis. In addition, differential effects on sunlit and shaded leaves associated with the canopy light environment contributed to this overall outcome when
integrated to the canopy level. Figure 6A-F shows the changes to instantaneous photosynthesis of the sunlit and shade leaf fractions throughout the day.

In the case of C\textsubscript{3}, Rubisco-limited (A\textsubscript{c,sun}) and electron-transport-limited (A\textsubscript{j,sun}) photosynthetic rates of the sunlit leaf fraction increased by an average of 2.6 and 7.2% over the diurnal cycle, respectively (Figure 6B). However, between 11 am and 3 pm, when the canopy had a high photosynthetic rate, the sunlit leaf fraction was Rubisco (A\textsubscript{c,sun}) limited. This interplay between A\textsubscript{c} and A\textsubscript{j} limitation throughout the day resulted in only 5.5% increase as opposed to the potential 7.2%. On the other hand, the shade leaf fraction increased by 7.7% over the diurnal cycle [all contributed by effects on electron-transport-limited rate (A\textsubscript{j})] (Figure 6C). Altogether, compared to a potential 7.2% increase in A\textsubscript{can,DAY}, A\textsubscript{c} limitation around noon reduced the potential increase in A\textsubscript{can,DAY} to 6.0%.

C\textsubscript{4} canopy photosynthesis was less responsive to changes in S\textsubscript{c/o} than C\textsubscript{3}, which was consistent with the notion that increasing S\textsubscript{c/o} in C\textsubscript{4} plants has less effect on photosynthesis as they have evolved CO\textsubscript{2}-concentrating mechanisms for enhanced photosynthesis. In the case of C\textsubscript{4} canopy photosynthesis, there was no interplay between Rubisco and electron transport limitations with all effects related to the latter (i.e. A\textsubscript{j}) (Figure 6E and F), and totalling to a 2.5% increase in A\textsubscript{can,DAY}.

**Rubisco activity and electron-transport rate**

There is evidence that Rubisco activity and electron transport capacity can vary among species, can respond to the prevailing environment, and be bioengineered [reviewed by Evans (2013)]. Putative changes in Rubisco activity and electron transport capacity can be implemented in the C\textsubscript{3} and C\textsubscript{4} photosynthesis models of DCaPS through changing the slope of the linear relationship between the maximum rate of Rubisco carboxylation (\(\chi\text{V}_{\text{c}}\)), the maximum rate of electron transport (\(\chi\text{j}\)) and specific leaf nitrogen; giving greater \(V_{\text{cmax}}\) and \(J_{\text{max}}\), respectively.

Here we examine diurnal canopy photosynthesis consequences of such variations.

The simulation of consequences on diurnal canopy photosynthesis of changes in \(V_{\text{cmax}}\) and \(J_{\text{max}}\) for C\textsubscript{3} and C\textsubscript{4} types are presented in Figure 6G-N. A\textsubscript{can,DAY} did not respond to increase in \(V_{\text{cmax}}\) for C\textsubscript{3} types because both the sunlit and shade leaf fractions were mostly electron transport (A\textsubscript{j}) limited in the reference scenario (Figure 6G) and any increase in Rubisco
activity ($A_c$) was not useful (Figure 6H). However, increasing $J_{\text{max}}$ could increase $A_{\text{can,DAY}}$ by 4.5%, which was attributed to higher electron-transport limited photosynthetic rate of the sunlit leaf fraction ($A_{\text{j,sun}}$) during early and late hours of the day (Figure 6I). The largest effect was when $V_{\text{c,max}}$ and $J_{\text{max}}$ were both increased by 20%, which gave a 9.5% increase in $A_{\text{can,DAY}}$. This shifted the whole diurnal photosynthetic rate higher (Figure 6J). It was apparent that the sunlit fraction of the canopy was more sensitive to these changes and contributed most to the higher canopy photosynthesis.

For C4 canopy photosynthesis, there was less interplay between Rubisco- and electron-transport-limited photosynthetic rate. C4 canopy photosynthesis was always electron-transport limited (Figure 6K). Hence, increase in Rubisco activity ($V_{\text{c,max}}$) had little or no effect on $A_{\text{can,DAY}}$ (Figure 6L). However, a 20% increase in maximum rate of electron transport ($J_{\text{max}}$) increased $A_{\text{can,DAY}}$ significantly (6%) (Figure 6M) and increasing both $J_{\text{max}}$ and $V_{\text{c,max}}$ simultaneously, increased $A_{\text{can,DAY}}$ by 8% (Figure 6N).

Implications for crop performance prediction – connecting biochemical photosynthesis models with crop models for seasonal simulations

Many crop models incorporate canopy photosynthesis as a key driver for crop growth for seasonal simulation. In some of these models, under well-watered conditions, canopy CO2 assimilation/biomass accumulation is based on the empirical Radiation Use Efficiency (RUE) approach, while others incorporate more detailed models of photosynthetic light response (PLR). Depending on the detail required for canopy photosynthesis simulation, either type of model can be used. However, the intrinsic empirical nature of these approaches makes it difficult to realistically model responses to manipulation of photosynthetic processes and environmental effects and so that often simple empirical indices are invoked to generate possible effects (Wu et al. 2016).

In this study, we have shown that the Diurnal Canopy Photosynthesis Simulator (DCaPS) can rationally simulate canopy photosynthetic rate responses to photosynthetic physiology, key environmental factors and crop status (e.g. light, $C_a$, $T_a$ and $SLN_{av}$). This provides confidence in incorporating DCaPS into crop growth and development models to drive above-ground canopy biomass accumulation in seasonal simulations. The capacity to connect with photosynthetic attributes makes DCaPS a valuable tool to improve the biological
functionality of crop models in terms of above-ground canopy biomass accumulation under well-watered conditions.

At first inspection, it may seem unduly complicated to introduce DCaPS into a crop model due to the parameterisation requirements at the biochemical/leaf level (Table 1). However, many are related to a small subset of key parameters, while others (e.g. temperature response parameters, Table 2) can be assigned *a priori* depending on the application of DCaPS. For example, the parameter values for kinetic properties of Rubisco (i.e. $K_c$, $K_o$, $V_{c_{\text{max}}}/V_{o_{\text{max}}}$) and their temperature responses are relatively conserved within C$_3$ species (von Caemmerer 2013). This means parameter values obtained from extensively studied model species, such as Arabidopsis and tobacco, can be used for C$_3$ crop species. Further, more comprehensive parameter values for C$_3$ (Braune *et al.* 2009) and C$_4$ (von Caemmerer 2000; Massad *et al.* 2007) crop species are also emerging. This leaves a small set of parameters (four and five parameters for C$_3$ and C$_4$, respectively) to be assigned as indicated in Table 1.

To facilitate connection with crop growth and development simulation models, DCaPS, which operates on a daily timescale, needs to be connected with environmental and crop canopy attribute data that vary throughout the growing season. These data, already used and output by some crop models, can be input on a daily frequency into DCaPS at the start of each daily simulation. Recall that DCaPS incorporates four key environmental parameters (radiation, $T_a$, $VPD_a$, $C_a$) and the three parameters for canopy attributes ($LAI_{\text{can}}$, $\beta$ (canopy-average leaf inclination relative to the horizontal) and $SLN_{\text{av}}$). Radiation, $T_a$, $VPD_a$, $LAI_{\text{can}}$ and $SLN_{\text{av}}$ can be connected with daily values supplied by crop models such as APSIM (Hammer *et al.* 2009; Hammer *et al.* 2010). This leaves $C_a$ and $\beta$ to be assigned. It would be reasonable to assume $C_a$ as a constant, while $\beta$ can be reasonably estimated if a spherical leaf-angle distribution is assumed for field crops [Eqn A26]. The design of DCaPS, which accepts daily values of environmental parameters and crop attributes allows convenient connection with crop models for seasonal simulation.

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temperature response of leaf photosynthesis as well as providing useful references, and the National eResearch Collaboration Tools and Resources (NECTAR) for providing a free web server for hosting dcaps.net.au.

Conflict of interest statement
The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.
### Table 1. Description of symbols used in the Diurnal Canopy Photosynthesis Simulator (DCaPS).

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
<th>Note</th>
<th>Value and reference</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_{\text{can,inst}}$</td>
<td>Instantaneous canopy CO$_2$ assimilation</td>
<td>μmol CO$_2$ m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td>A73</td>
</tr>
<tr>
<td>$A_{\text{can,DAY}}$</td>
<td>Diurnal canopy CO$_2$ assimilation</td>
<td>μmol CO$_2$ m$^{-2}$ ground day$^{-1}$</td>
<td></td>
<td></td>
<td>A73</td>
</tr>
<tr>
<td>$B$</td>
<td>Conversion ratio combines factors allowing for biochemical conversion and maintenance respiration</td>
<td>g biomass (g CO$_2$)$^{-1}$</td>
<td>A</td>
<td>0.41 (wheat and sorghum) (Sinclair and Horie 1989)</td>
<td>A74</td>
</tr>
<tr>
<td>$BIO_{\text{total,DAY}}$</td>
<td>Daily total biomass increment</td>
<td>g biomass m$^{-2}$ ground day$^{-1}$</td>
<td></td>
<td></td>
<td>A74</td>
</tr>
<tr>
<td>$P_{\text{shoot}}$</td>
<td>Fraction of above-ground (shoot) biomass to the total (shoot + root) biomass</td>
<td>g shoot biomass (g total biomass)$^{-1}$</td>
<td>A</td>
<td></td>
<td>A74</td>
</tr>
<tr>
<td>$BIO_{\text{shoot,DAY}}$</td>
<td>Daily above-ground canopy (shoot) biomass increment</td>
<td>g biomass m$^{-2}$ ground day$^{-1}$</td>
<td>E</td>
<td></td>
<td>A74</td>
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<tr>
<td>$k_{\text{DAY}}$</td>
<td>Canopy solar radiation extinction coefficient on daily basis</td>
<td></td>
<td></td>
<td></td>
<td>A78</td>
</tr>
<tr>
<td>$R\text{AD}_{\text{DAY}}$</td>
<td>Total daily intercepted solar radiation</td>
<td>MJ m$^{-2}$ ground day$^{-1}$</td>
<td></td>
<td></td>
<td>A76</td>
</tr>
<tr>
<td>$R\text{UE}_{\text{DAY}}$</td>
<td>Radiation use efficiency on daily basis</td>
<td>g biomass MJ$^{-1}$</td>
<td></td>
<td></td>
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### Environmental Parameters

<table>
<thead>
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<th>Units</th>
<th>Note</th>
<th>Value and reference</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_s$</td>
<td>Total daily extra-terrestrial solar radiation</td>
<td>MJ m$^{-2}$ ground day$^{-1}$</td>
<td></td>
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</tr>
<tr>
<td>$S_r$</td>
<td>Total daily incident solar radiation</td>
<td>MJ m$^{-2}$ ground day$^{-1}$</td>
<td></td>
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<td>A4</td>
</tr>
<tr>
<td>$R\text{ATIO}$</td>
<td>Atmospheric transmission ratio</td>
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<td>A,D</td>
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</tr>
<tr>
<td>$sc$</td>
<td>Solar constant</td>
<td>J m$^{-2}$ ground s$^{-1}$</td>
<td>A</td>
<td>1360</td>
<td>A5</td>
</tr>
<tr>
<td>$Lat$</td>
<td>Latitude in radians (negative in the southern hemisphere)</td>
<td>radians</td>
<td>A</td>
<td></td>
<td>A5</td>
</tr>
<tr>
<td>$Rl$</td>
<td>Radius vector</td>
<td>radians</td>
<td>A</td>
<td></td>
<td>A6</td>
</tr>
<tr>
<td>$Di$</td>
<td>Solar declination</td>
<td>radians</td>
<td>A</td>
<td></td>
<td>A8</td>
</tr>
<tr>
<td>$Wt^\circ$</td>
<td>Sunset hour-angle</td>
<td>°</td>
<td>A</td>
<td></td>
<td>A7</td>
</tr>
<tr>
<td>$Ll$</td>
<td>Day length</td>
<td>hr</td>
<td>A</td>
<td></td>
<td>A10</td>
</tr>
<tr>
<td>$D\text{AY}$</td>
<td>Day of year</td>
<td></td>
<td>A,D</td>
<td></td>
<td>A12</td>
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<tr>
<td>$t_{\text{frac}}$</td>
<td>$t$ as a fraction of $Ll$</td>
<td></td>
<td></td>
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<tr>
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<td>Time of sunrise</td>
<td>hr</td>
<td>A</td>
<td></td>
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<tr>
<td>$t_{\text{sunset}}$</td>
<td>Time of sunset</td>
<td>hr</td>
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<td>$\alpha_{\text{sun}}$</td>
<td>Angle of solar elevation</td>
<td>radians or degree</td>
<td>A</td>
<td></td>
<td>A9</td>
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<tr>
<td>$T_a$</td>
<td>Air temperature</td>
<td>°C</td>
<td>A</td>
<td></td>
<td>A15</td>
</tr>
<tr>
<td>$T_{a,max}$</td>
<td>Maximum $T_a$ of $D\text{AY}$</td>
<td>°C</td>
<td>A,D</td>
<td></td>
<td>A15</td>
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<tr>
<td>$T_{a,min}$</td>
<td>Minimum $T_a$ of $D\text{AY}$</td>
<td>°C</td>
<td>A,D</td>
<td></td>
<td>A15</td>
</tr>
<tr>
<td>$m$</td>
<td>Amount of time since time of minimum temperature</td>
<td>hr</td>
<td>A</td>
<td></td>
<td>A15</td>
</tr>
<tr>
<td>$n$</td>
<td>Amount of time since $t_{\text{sunset}}$</td>
<td>hr</td>
<td>A</td>
<td></td>
<td>A15</td>
</tr>
<tr>
<td>$x_{\text{lag}}$</td>
<td>Lag coefficient for the maximum temperature from $t_{\text{sunrise}}$</td>
<td>A</td>
<td>1.8</td>
<td>(Parton and Logan 1981)</td>
<td>A15</td>
</tr>
<tr>
<td>$y_{\text{lag}}$</td>
<td>Lag coefficient for the night-time temperature from $t_{\text{sunrise}}$</td>
<td>A</td>
<td>2.2</td>
<td>(Parton and Logan 1981)</td>
<td>A15</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td></td>
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</tr>
<tr>
<td>$z_{\text{lag}}$</td>
<td>Lag coefficient for the minimum temperature from $T_{\text{sunrise}}$</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$\text{VPD}_{\text{a}}$</td>
<td>Air vapour pressure deficit, kPa</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$C_{\text{a}}$</td>
<td>Air CO$_2$ partial pressure, $\mu$bar</td>
<td></td>
<td></td>
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<td></td>
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<tr>
<td>$O_{\text{a}}$</td>
<td>Air O$_2$ partial pressure, $\mu$bar</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_s$</td>
<td>Total incident solar radiation, MJ m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{dir}}$</td>
<td>Incident direct radiation, MJ m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{dif}}$</td>
<td>Incident diffuse radiation, MJ m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{PAR}}$</td>
<td>Total incident photosynthetic active radiation, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{PAR},\text{dir}}$</td>
<td>Direct incident photosynthetic active radiation, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{PAR},\text{dif}}$</td>
<td>Diffuse incident photosynthetic active radiation, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{abs,can}}$</td>
<td>Absorbed PAR by the canopy, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{abs,sh}}$</td>
<td>Absorbed PAR by the shaded fraction of the canopy, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{abs,sun}}$</td>
<td>Absorbed PAR by the sunlit fraction of the canopy, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_{\text{PAR},\text{dir}} + I_{\text{PAR},\text{dif}}$</td>
<td>Total incident PAR radiation, $\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
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</table>

**Canopy Attribute and Architecture Parameters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{LAI}_{\text{can}}$</td>
<td>Canopy leaf area index, m$^2$ leaf m$^{-2}$ ground</td>
</tr>
<tr>
<td>$\text{LAI}_{\text{sun}}$</td>
<td>LAI of the sunlit leaf fraction, m$^2$ leaf m$^{-2}$ ground</td>
</tr>
<tr>
<td>$\text{LAI}_{\text{sh}}$</td>
<td>LAI of the shade leaf fraction, m$^2$ leaf m$^{-2}$ ground</td>
</tr>
<tr>
<td>$L$</td>
<td>Cumulative LAI from the top of canopy, m$^2$ leaf m$^{-2}$ ground</td>
</tr>
<tr>
<td>$k_b'$</td>
<td>Direct and scattered direct PAR extinction coefficient</td>
</tr>
<tr>
<td>$k_d'$</td>
<td>Diffuse and scattered diffuse PAR extinction coefficient</td>
</tr>
<tr>
<td>$k_b$</td>
<td>Direct radiation extinction coefficient</td>
</tr>
<tr>
<td>$k_d$</td>
<td>Diffuse PAR extinction coefficient</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Leaf-level scattering coefficient for PAR</td>
</tr>
<tr>
<td>$\rho_{\text{dn}}$</td>
<td>Canopy-level reflection coefficient for direct PAR</td>
</tr>
<tr>
<td>$\rho_{\text{dt}}$</td>
<td>Canopy-level reflection coefficient for diffuse PAR</td>
</tr>
<tr>
<td>$G$</td>
<td>Leaf shadow projection coefficient</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Canopy-average leaf inclination relative to the horizontal, radians</td>
</tr>
<tr>
<td>$T_1$</td>
<td>Leaf temperature, °C</td>
</tr>
</tbody>
</table>

Note: Values in parentheses indicate the source of data or study (de Pury and Farquhar 1997)
Canopy Nitrogen Status Parameters

- **SLN<sub>av</sub>** Specific leaf nitrogen averaged over the whole canopy, g N m<sup>-2</sup> leaf
  - 1.45 (wheat) (de Purry and Farquhar 1997), 1.36 (sorghum) (van Oosterom et al. 2010)

- **SLN<sub>ratio_top</sub>** Ratio of SLN<sub>o</sub> to SLN<sub>av</sub>, g N m<sup>-2</sup> leaf
  - 1.32 (wheat) (de Purry and Farquhar 1997), 1.30 (sorghum) (van Oosterom et al. 2010)

- **SLN<sub>o</sub>** SLN at the top of canopy, g N m<sup>-2</sup> leaf

- **N(L)** SLN at L, mmol N m<sup>-2</sup> leaf

- **N<sub>o</sub>** SLN at the top of canopy, mmol N m<sup>-2</sup> leaf

- **N<sub>b</sub>** Base SLN at or below which leaf photosynthesis = 0, mmol N m<sup>-2</sup> leaf
  - 25 (wheat) (de Purry and Farquhar 1997), 14 (sorghum) (Sinclair and Horie 1989)

- **k<sub>n</sub>** Coefficient of nitrogen allocation through canopy

Photosynthesis Parameters

- **χ<sub>V</sub>** Slope of linear relationship between <i>V</i><sub>max</sub> per leaf are at 25°C and N, μmol CO<sub>2</sub> mmol<sup>-1</sup> N s<sup>-1</sup> B
  - 1.16 (de Purry and Farquhar 1997) (wheat), 0.35 (sorghum) (Massad et al. 2007)
  - 24 (wheat) (de Purry and Farquhar 1997)

- **χ<sub>J</sub>** Slope of linear relationship between <i>J</i><sub>max</sub> per leaf are at 25°C and N, μmol CO<sub>2</sub> mmol<sup>-1</sup> N s<sup>-1</sup> B
  - 2.4 (wheat) (de Purry and Farquhar 1997), 2.4 (sorghum) (Massad et al. 2007)

- **χ<sub>R</sub>** Slope of linear relationship between <i>R</i><sub>d</sub> per leaf are at 25°C and N, μmol CO<sub>2</sub> mmol<sup>-1</sup> N s<sup>-1</sup> B
  - 0.01<sub>SV</sub> (wheat) (de Purry and Farquhar 1997), 0 (sorghum) (Massad et al. 2007)

- **χ<sub>P</sub>** Slope of linear relationship between <i>V</i><sub>pmax</sub> per leaf are at 25°C and N, μmol CO<sub>2</sub> mmol<sup>-1</sup> N s<sup>-1</sup> B
  - 4.1 (sorghum) (Massad et al. 2007)

- **<i>V</i><sub>cm</sub><sup>ax</sup>** Maximum rate of Rubisco carboxylation, μmol CO<sub>2</sub> m<sup>-2</sup> ground s<sup>-1</sup> Table 2

- **<i>J</i><sub>max</sub>** Maximum rate of electron transport, μmol CO<sub>2</sub> m<sup>-2</sup> ground s<sup>-1</sup> Table 2

- **<i>R</i><sub>d</sub>** Leaf day respiration, μmol CO<sub>2</sub> m<sup>-2</sup> ground s<sup>-1</sup> Table 2
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{mt}$</td>
<td>Mesophyll mitochondrial respiration</td>
<td>$\mu$mol CO$_2$ m$^{-2}$ ground s$^{-1}$</td>
<td>C$_4$ Caemmerer 2000</td>
</tr>
<tr>
<td>$K_c$</td>
<td>Michaelis-Menten constant of Rubisco for CO$_2$</td>
<td>$\mu$bar</td>
<td>Table 2</td>
</tr>
<tr>
<td>$K_o$</td>
<td>Michaelis-Menten constant of Rubisco for O$_2$</td>
<td>$\mu$bar</td>
<td>Table 2</td>
</tr>
<tr>
<td>$A_c$</td>
<td>RuBP-saturated (or Rubisco-limited) net CO$_2$ assimilation rate</td>
<td>$\mu$mol m$^{-2}$ ground s$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$A_o$</td>
<td>RuBP-regeneration-limited (or electron-transport-limited) net CO$_2$ assimilation rate</td>
<td>$\mu$mol m$^{-2}$ ground s$^{-1}$</td>
<td></td>
</tr>
<tr>
<td>$\Gamma_c$</td>
<td>CO$_2$ compensation point in the absence of $R_d$</td>
<td>$\mu$bar</td>
<td>A52</td>
</tr>
<tr>
<td>$\gamma_c$</td>
<td>Half the reciprocal of $S_{\text{co2}}$</td>
<td>$\bar{\text{bar}}$</td>
<td>$0.5S_{\text{co2}}$</td>
</tr>
<tr>
<td>$S_{\text{co2}}$</td>
<td>Relative CO$_2$/O$_2$ specificity of Rubisco</td>
<td>$\text{bar} \text{bar}^{-1}$</td>
<td>A53</td>
</tr>
<tr>
<td>$V_{\text{carb}}/V_{\text{max}}$</td>
<td>Carboxylation to maximum rate of Rubisco oxygenation</td>
<td></td>
<td>Table 2 A53</td>
</tr>
<tr>
<td>$J$</td>
<td>Potential electron transport rate</td>
<td>$\mu$mol e$^-$ m$^{-2}$ ground s$^{-1}$</td>
<td>A46</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Empirical curvature factor</td>
<td>A</td>
<td>0.7 (de Pury and Farquhar 1997) A46</td>
</tr>
<tr>
<td>$f$</td>
<td>Spectral correction factor</td>
<td>A</td>
<td>0.15 (de Pury and Farquhar 1997) A46</td>
</tr>
<tr>
<td>$I_2$</td>
<td>PAR absorbed by Photosystem II</td>
<td>$\mu$mol PAR m$^{-2}$ ground s$^{-1}$</td>
<td>A45</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Fraction of PSII activity in the bundle sheath</td>
<td></td>
<td>C$_4$ 0.1 (Yin and Struik 2009) A56</td>
</tr>
<tr>
<td>$V_p$</td>
<td>Rate of PEP carboxylation</td>
<td>$\mu$mol CO$_2$ m$^{-2}$ ground s$^{-1}$</td>
<td>C$_4$ A58</td>
</tr>
<tr>
<td>$V_{\text{max}}$</td>
<td>Maximum PEP carboxylase activity</td>
<td>$\mu$mol CO$_2$ m$^{-2}$ ground s$^{-1}$</td>
<td>C$_4$ Table 2</td>
</tr>
<tr>
<td>$K_p$</td>
<td>Michaelis-Menten constant of PEP carboxylase for CO$_2$</td>
<td>$\mu$bar</td>
<td>C$_4$ Table 2</td>
</tr>
<tr>
<td>$V_{\text{pr,leaf}}$</td>
<td>PEP regeneration rate per leaf area</td>
<td>$\mu$mol CO$_2$ m$^{-2}$ leaf s$^{-1}$</td>
<td>A,C$_4$ Caemmerer 2000</td>
</tr>
<tr>
<td>$V_{\text{pr}}$</td>
<td>PEP regeneration rate</td>
<td>$\mu$mol CO$_2$ m$^{-2}$ ground s$^{-1}$</td>
<td>C$_4$ A58</td>
</tr>
<tr>
<td>$J_{\text{t}}$</td>
<td>Potential electron transport rate (symbol for C$_4$)</td>
<td>$\mu$mol e$^-$ m$^{-2}$ ground s$^{-1}$</td>
<td>C$_4$ A46</td>
</tr>
<tr>
<td>$x$</td>
<td>Fraction of electron transport partitioned to mesophyll chloroplasts</td>
<td></td>
<td>A,C$_4$ Caemmerer 2000 A59</td>
</tr>
</tbody>
</table>

**CO$_2$ Diffusion Parameters**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_i$</td>
<td>Intercellular airspace CO$_2$ partial pressure</td>
<td>$\mu$bar</td>
<td></td>
</tr>
<tr>
<td>$C_m$</td>
<td>Mesophyll CO$_2$ partial pressure</td>
<td>$\mu$bar</td>
<td>C$_4$ A57, A60</td>
</tr>
<tr>
<td>$C_c$</td>
<td>Chloroplastic CO$_2$ partial pressure at the site of Rubisco carboxylation</td>
<td>$\mu$bar</td>
<td>A51, A54</td>
</tr>
<tr>
<td>$C_s$</td>
<td>Bundle-sheath CO$_2$ partial pressure</td>
<td>$\mu$bar</td>
<td>C$_4$ A55, A59</td>
</tr>
<tr>
<td>$O_i$</td>
<td>O$_2$ partial pressure inside C$_3$ and C$_4$ leaves</td>
<td>$\mu$bar</td>
<td>O$_i$</td>
</tr>
<tr>
<td>$O_c$</td>
<td>Chloroplastic O$_2$ partial pressure at the site of Rubisco carboxylation</td>
<td>$\mu$bar</td>
<td>O$_i$</td>
</tr>
<tr>
<td>$O_m$</td>
<td>Mesophyll O$_2$ partial pressure</td>
<td>$\mu$bar</td>
<td>C$_4$ O$_i$ A56</td>
</tr>
<tr>
<td>$O_s$</td>
<td>Bundle-sheath O$_2$ partial pressure</td>
<td>$\mu$bar</td>
<td>C$_4$ A56</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
<td>Unit</td>
<td>Value</td>
</tr>
<tr>
<td>-----------</td>
<td>-------------</td>
<td>------</td>
<td>-------</td>
</tr>
<tr>
<td>$a$</td>
<td>Slope of linear relationship between $C_i/C_a$ and $VPD_a$</td>
<td>kPa$^{-1}$</td>
<td>-0.12 (C$_3$), -0.19 (C$_4$) (Zhang and Nobel 1996)</td>
</tr>
<tr>
<td>$b$</td>
<td>Intercept of linear relationship between $C_i/C_a$ and $VPD_a$</td>
<td></td>
<td>0.9 (C$_3$), 0.84 (C$_4$) (Zhang and Nobel 1996)</td>
</tr>
<tr>
<td>$C_i/C_a$</td>
<td>Ratio of $C_i$ to $C_a$</td>
<td></td>
<td>A (Table 2)</td>
</tr>
<tr>
<td>$g_m$</td>
<td>Mesophyll conductance for CO$_2$</td>
<td>mol CO$_2$ m$^{-2}$ ground s$^{-1}$ bar$^{-1}$</td>
<td>B (von Caemmerer 2000)</td>
</tr>
<tr>
<td>$g_s$</td>
<td>Bundle-sheath conductance for CO$_2$</td>
<td>mol CO$_2$ m$^{-2}$ ground s$^{-1}$ bar$^{-1}$</td>
<td>C$_4$</td>
</tr>
</tbody>
</table>

**Table 2: DCaPS input parameters that could be assigned a priori; B: DCaPS input parameters that require calibration for different crop species; D: connector with crop models; C$_4$: parameters specific to the C$_4$ photosynthesis model; E: DCaPS output to crop models; blank in the note column means symbol is a calculated variable.**
Table 2. C₃ and C₄ temperature response parameters used in equations 1 and 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>C₃</th>
<th>C₄</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$P_{25}$ $c$ (dimensionless)</td>
<td>$b$ (K)</td>
</tr>
<tr>
<td>$K_c$</td>
<td>μbar</td>
<td>272.4¹</td>
<td>32.7¹</td>
</tr>
<tr>
<td>$K_o$</td>
<td>μbar</td>
<td>165800³</td>
<td>9.6¹</td>
</tr>
<tr>
<td>$V_{cmax}/V_{cmax}$</td>
<td>-</td>
<td>4.6¹</td>
<td>13.2¹</td>
</tr>
<tr>
<td>$V_{cmax}$</td>
<td>μmol m⁻² s⁻¹</td>
<td>A</td>
<td>26.4²</td>
</tr>
<tr>
<td>$R_d$</td>
<td>μmol m⁻² s⁻¹</td>
<td>A</td>
<td>18.7²</td>
</tr>
<tr>
<td>$K_p$</td>
<td>μbar</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$V_{pmax}$</td>
<td>μmol m⁻² s⁻¹</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$P_{25}$</td>
<td>$T_{opt}$ (°C)</td>
</tr>
<tr>
<td>$J_{max}$</td>
<td>μmol m⁻² s⁻¹</td>
<td>A</td>
<td>28.8³</td>
</tr>
<tr>
<td>$g_m$</td>
<td>μmol m⁻² s⁻¹ bar⁻¹</td>
<td>0.55</td>
<td>34.3¹</td>
</tr>
</tbody>
</table>

A: variable. -: not applicable (see text). References: ¹ (Bernacchi et al. 2002), ² (Bernacchi et al. 2001), ³ (Farquhar et al. 1980), ⁴ (Boyd et al. 2015), ⁵ (Massad et al. 2007).
Figure 1. Schematic of the Diurnal Canopy Photosynthesis Simulator (DCaPS). Model inputs are categorised into environment, canopy attributes and architecture, canopy nitrogen status, CO$_2$ diffusion, photosynthetic, and temperature response parameters. Model outputs are diurnal environment variables, diurnal canopy photosynthesis and daily above-ground canopy biomass increment. The two-way arrow between the CO$_2$ diffusion model and the biochemical models indicates that the models are coupled and solved simultaneously for the chloroplastic CO$_2$ partial pressure ($C_c$) and photosynthesis.

Symbols: $\text{RATIO}$, atmospheric transmission ratio for incident solar radiation; $\text{VPD}_a$, air vapour pressure deficit; PAR, photosynthetic active radiation; $\text{SLN}_{\text{av}}$, canopy-average specific leaf nitrogen; $\text{SLN}_{\text{ratio\_top}}$, ratio of SLN at the top of canopy to $\text{SLN}_{\text{av}}$; $T_l$, leaf temperature; $g_m$, mesophyll conductance for CO$_2$; $g_{bs}$, bundle-sheath conductance for CO$_2$; $O_l$, O$_2$ partial pressure inside leaves. The SLN canopy profile is used to calculate parameters in bold font. Comprehensive lists of the photosynthetic parameters are given in Tables 1 and 2.
Figure 2. Diurnal net C\textsubscript{3} (upper panels) and C\textsubscript{4} (lower panels) canopy photosynthesis with various combinations of canopy attributes: leaf area index (\textit{LAI}_{\text{can}}) of 2, 4 or 8 and canopy-average leaf inclination relative to the horizontal (\(\beta\)) of 40\(^\circ\) (A and C) or 80\(^\circ\) (B and D). In all four panels, the lower, middle and top curves show results for \textit{LAI}_{\text{can}} of 2, 4 and 8, respectively. Default values of other model parameters are given in Tables 1 and 2.
Figure 3. Relative net \( \text{C}_3 \) (dashed curves) and \( \text{C}_4 \) (solid curves) daily canopy photosynthesis (\( A_{\text{can,DAY}} \)) and Radiation Use Efficiency on a daily basis (\( \text{RUE}_{\text{DAY}} \)) in response to air \( \text{CO}_2 \) and temperature. \( A_{\text{can,DAY}} \) or \( \text{RUE}_{\text{DAY}} \) curves were normalised to their respective values at an air \( \text{CO}_2 \) partial pressure (\( C_a \)) = 360 μbar, respectively. Days were categorised as hot (14–28°C), average (7–21°C) or cold (0–14°C) for winter wheat crops; temperatures were not assigned to \( \text{C}_4 \) curves due to their small response to \( C_a \). The triangle indicates a 28% increase in \( A_{\text{can,DAY}} \) at an average \( C_a \) of 540 μbar on hot days, relative to that at \( C_a = 360 \mu\text{bar} \); the circle indicates a 19% increase in relative \( A_{\text{can,DAY}} \) increase on average days at the same average \( C_a \). These relative increases were taken from (Ainsworth and Long 2005). Default values of other model parameters are given in Tables 1 and 2.
Figure 4. Radiation Use Efficiency on a daily basis of C\textsubscript{3} (dashed curve) and C\textsubscript{4} (solid curve) canopy in response to temperature. \( \text{RUE}_{\text{DAY}} \) is plotted against average daily air temperature, which is calculated by averaging the daily maximum \( T_{a,max} \) and minimum \( T_{a,min} \) air temperatures; \( T_{a,max} = T_{a,min} + 15 \) with \( T_{a,min} = 0–20^\circ \text{C} \) for C\textsubscript{3} and 10–25°C for C\textsubscript{4}. Solid curve 1 was simulated for a dwarf hybrid sorghum with the slope of the linear relationship between the maximum rate of Rubisco carboxylation (\( \chi_{Vc} \)), maximum rate of electron transport (\( \chi_I \)), maximum PEP carboxylase activity (\( \chi_{VP} \)) and specific leaf nitrogen of 0.5, 2.4 and 1.0 μmol CO\textsubscript{2} (mmol N)\textsuperscript{-1} s\textsuperscript{-1}, respectively; solid curve 2 was simulated for maize and tall hybrid sorghum with \( \chi_{Vc}, \chi_I \) and \( \chi_{VP} \) of 1.0, 4.0 and 2.0 μmol CO\textsubscript{2} (mmol N)\textsuperscript{-1} s\textsuperscript{-1}, respectively. Default values of other model parameters are given in Tables 1 and 2.
Figure 5. Radiation Use Efficiency on a daily basis for (A) C₃ and (B) C₄ canopy in response to specific leaf nitrogen and solar radiation levels. RUE$_{\text{DAY}}$ is plotted against canopy-average specific leaf nitrogen (SLN$_{av}$). Curves 1 (lowest curve), 2 and 3 (highest curve) are obtained by setting $\text{RATIO}$ to 0.75 (clear sky), 0.55 and 0.35 (heavy cloud cover), respectively, which changes the amount of incident radiation (curve 1 greatest) and the proportion that is diffuse (curve 3 greatest). This order applies to panel B as well. Dotted curves in panel B show simulated RUE$_{\text{DAY}}$ for a standard C₄ crop (e.g. maize) with $\chi_V$, $\chi_I$ and $\chi_P$ of 1.0, 4.0 and 2.0 $\mu$mol CO₂ (mmol N)$^{-1}$ s$^{-1}$, respectively. Default values of other model parameters are given in Tables 1 and 2.
Figure 6. Dirunal $C_3$ and $C_4$ canopy photosynthesis and photosynthetic changes. The top two rows ($C_3$ and $C_4$, respectively) show % changes in diurnal canopy photosynthesis with 25% increase in the relative CO$_2$/O$_2$ specificity of Rubisco ($S_{c/o}$). A and D: reference net $A_{\text{inst}}$ at default $S_{c/o}$; B and E: % changes in net $A_{\text{inst}}$ for the sunlit leaf fraction of the canopy; C and F: % changes in net $A_{\text{inst}}$ for the shade leaf fraction. The bottom two rows ($C_3$ and $C_4$, respectively) show changes in diurnal canopy photosynthesis with various Rubisco activity ($V_{\text{cmax}}$) and/or electron transport capacity ($J_{\text{max}}$). G and K: reference net $A_{\text{inst}}$ with default values; H and L: $V_{\text{cmax}}$ increased by 20%; I and M: $J_{\text{max}}$ increased by 20%; J and N: $V_{\text{cmax}}$ and $J_{\text{max}}$ both increased by 20%. Solid and dotted curves show values for the sunlit ($A_{\text{sun}}$) and shade ($A_{\text{sh}}$) leaf fractions of the canopy, respectively; grey and black colour coding are for Rubisco-limited ($A_c$) and electron-transport limited ($A_j$) photosynthetic rate, respectively. The $A_{c,sh}$ curve is removed from H, I, J, L, M and N except in G and K where it is plotted using the right hand ordinate (indicated by arrows). Filled areas indicate CO$_2$ assimilation rate or its % change in the sunlit leaf fraction and
patterned areas indicate the same for the shade leaf fraction. For each leaf fraction, photosynthetic rate is given by the minimum of $A_c$ and $A_j$. Note that diurnal canopy photosynthesis ($A_{\text{can, DAY}}$; see text) is obtained by summing the photosynthetic rate of the two leaf fractions, integrate hourly and sum over the diurnal period. Default values of other model parameters are given in Tables 1 and 2.
References


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