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Supplementary Material: *Functional Plant Biology*

Supplementary Material

Simulating daily field crop canopy photosynthesis: an integrated software package

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APPENDIX 1: <u>D</u>IURNAL <u>CA</u>NOPY <u>P</u>HOTOSYNTHESIS <u>S</u>IMULATOR (<u>DCAPS</u>) - MODEL DOCUMENTATION

This document explains in detail the modelling and calculations in DCaPS. The source code of the DCaPS web-based application (v1.0) is available at https://github.com/QAAFI/DCaPS.git. Materials are categorised into sections, which reflect the model components shown in Figure 1 of the main text. Please refer to Table S1 and S2 (replicates of Table 1 and 2 in the main text, respectively) for parameter and variable descriptions.

Diurnal incident direct and diffuse radiation

The total incident solar radiation (I_o, MJ m^{-2} s^{-1}) at any time (t) consists of direct (I_{dir}, MJ m^{-2} s^{-1}) and diffuse (I_{dif}, MJ m^{-2} s^{-1}) components. They depend on latitude (*Lat*, radians), day of year (*DAY*), time of day (t) and the atmospheric transmission ratio (RATIO) (Hammer and Wright 1994). RATIO is taken as 0.75 as it ranges from 0.7 to 0.8 for clear skies. Under such conditions with a *RATIO* of about 0.75 (Hammer and Wright 1994), 23% of S_g is diffuse radiation (Spitters 1986), which represents 17% of solar insolation (S_o). Because the 17% atmospheric transmission ratio of diffuse radiation is insensitive to solar elevation and cloud conditions (Collares-Pereira and Rabl 1979), this proportion can be used for any *Lat*, *DAY* and *RATIO* (Hammer and Wright 1994). Hence, I_{dif} can be simply calculated from extra-terrestrial radiation, which depends only on the solar constant (sc, 1360 J m^{-2} s^{-1}) and solar elevation angle (α_{sun}) (Hammer and Wright 1994):

$$I_{\mathrm{dif}} = 0.17 \times sc \times \sin(\alpha_{\mathrm{sun}})/1000000 \qquad \text{(A1)}$$

The diurnal pattern of atmospheric transmission of direct radiation is more complex, so we obtain I_{dir} by difference once I_o is calculated (Hammer and Wright 1994):

$$I_{\mathrm{dir}} = I_{\mathrm{o}} - I_{\mathrm{dif}} \qquad \text{(A2)}$$

However, if $I_o < I_{dif}$ then $I_o = I_{dif}$ and $I_{dir} = 0$ (Hammer and Wright 1994).

The instantaneous solar radiation above the canopy (I_o, MJ m^{-2} s^{-1}) is estimated from the daily integral of solar radiation reaching the ground (S_g, MJ m^{-2} day^{-1}), the daylength (Ll, hours)), and the time of day as a fraction of Ll (t_{frac}) (Charles-Edwards 1986):

$$I_{\mathrm{o}} = S_{\mathrm{g}} \pi sin(\pi t_{\mathrm{frac}})/(2L\mathrm{l} \times 3600) \qquad \text{(A3)}$$

where the unit m^{-2} is referring to per ground area unless stated otherwise.

The daily integral of solar radiation reaching the ground (S_g) is calculated as the product of daily extra-terrestrial radiation (S_o, MJ m^{-2} day^{-1}) by atmospheric transmission ratio (RATIO) (Hammer and Wright 1994):

$$S_{\mathrm{g}} = S_{\mathrm{o}} \times \mathrm{RATIO} \tag{A4}$$

The daily extra-terrestrial radiation is obtained from day of the year (determines various parameters related to sun's geometry) and the latitude via the following equation (Brock 1981):

$$S_{\mathrm{o}} = \frac{24}{\pi}\frac{sch}{R\mathrm{l}^2}\left(W\mathrm{l}^{\circ}\,\frac{\pi}{180}\sin Lat \sin D\mathrm{l} + \sin W\mathrm{l} \cos Lat \cos D\mathrm{l}\right) \tag{A5}$$

where *sch* (4896000 J m^{-2} hr^{-1}) is the solar constant in energy units per hour, *R*l is the radius vector of the Earth, *W*l° is the sunset hour-angle in degrees, *Lat* is latitude (negative in the southern hemisphere), *D*l is solar declination.

The radius vector (*R*l), expressing the ellipticity of the Earth's distance to the Sun, depends on the day of the year (*DAY*) and is given by:

$$R\mathrm{l} = 1/\sqrt{\{1 + [0.033\cos(360DAY/365)]\}} \tag{A6}$$

Where DAY day of the year (the number of days after 1 January).

The angle between the setting Sun and the south point, which depends on the latitude, is the sunset hour-angle (given in degrees):

$$W\mathrm{l}^{\circ} = \mathrm{acos}[-(\tan Lat \tan D\mathrm{l})] \times \frac{180}{\pi} \tag{A7}$$

The declination of the Earth is the angular distance at solar noon between the Sun and the Equator, named the solar declination, is dependent on *DAY* and is given by:

$$D\mathrm{l} = 23.45\sin[2\pi\,(248 + DAY)/365] \times \frac{\pi}{180} \tag{A8}$$

Cosine of the solar elevation angle:

$$\sin(\alpha_{\mathrm{sun}}) = \sin LAT \sin D\mathrm{l} + \cos LAT \cos D\mathrm{l} \cos\left[L\mathrm{l} \times (t_{\mathrm{frac}} - 0.5) \times \frac{\pi}{12}\right] \tag{A9}$$

where *L*l (hour) is day length and t_{frac} is fraction of day passed at *t* from the time of sunrise. The day length is given by:

$$L\mathrm{l} = (W\mathrm{l}^{\circ}/15) \times 2 \tag{A10}$$

where *W*l° (degrees) is the sunset hour-angle and is given by:

$$Wl° = \mathrm{acos}[-(\tan DAY \tan Dl)] \times \frac{\pi}{180} \quad \text{(A11)}$$

Fraction of day (t_{frac}) is given by:

$$t_{\mathrm{frac}} = [t - (12 - 0.5Ll)]/Ll \quad \text{(A12)}$$

Eqn A12 assumes that midday always occurs at 12:00 pm. Time at sunrise (t_{sunrise}) and sunset (t_{sunset}) are given by:

$$t_{\mathrm{sunrise}} = 12 - 0.5 \times Ll \quad \text{(A13)}$$

$$t_{\mathrm{sunset}} = 12 + 0.5 \times Ll \quad \text{(A14)}$$

Daily air temperature

Using slightly modified methods from those developed by Parton and Logan (1981), diurnal air temperature at time t is calculated for both day-time and night-time temperatures using the following equations:

$$T_{\mathrm{a}} = \begin{cases} \left(T_{\mathrm{a,max}} - T_{\mathrm{a,min}}\right) \sin\left(\frac{\pi m}{L1 + 2x_{\mathrm{lag}}}\right) + T_{\mathrm{a,min}}, & t_{\mathrm{Tmin}} \leq t < t_{\mathrm{sunset}} \\ T_{\mathrm{a,min}} + \left(T_{\mathrm{sunset}} - T_{\mathrm{a,min}}\right) exp\left(-\frac{n y_{\mathrm{lag}}}{(24 - L1)}\right), & t < t_{\mathrm{Tmin}}, t \geq t_{\mathrm{sunset}} \end{cases} \quad \text{(A15)}$$

where $T_{\mathrm{a,max}}$ and $T_{\mathrm{a,min}}$ are the maximum and minimum air temperature for *DAY*, T_{sunset} is the air temperature at sunset (calculated using day-time formula above), t_{Tmin} is the time at the minimum temperature, calculated by $t_{\mathrm{Tmin}} = t_{\mathrm{sunrise}} + z_{\mathrm{lag}}$, m is the amount of time since t_{Tmin}, which is used between t_{Tmin} and t_{sunset}; n is the amount of time since t_{sunset}, which is used between t_{sunset} and t_{Tmin}. The parameters x_{lag}, y_{lag}, and z_{lag} are the lag coefficient for the maximum temperature, the night-time temperature coefficient and the lag of minimum temperature from the time of sunrise, respectively. The default values for x_{lag}, y_{lag}, and z_{lag} are 1.8, 2.2 and 1 respectively.

Diurnal air vapour pressure deficit

Vapour Pressure Deficit of the air (VPD_{a}, kPa) is calculated by the difference between saturated vapour pressure of the air (SVP_{a}) at T_{a} and the dew-point vapour pressure (SVP_{d}) (Goudriaan and van Laar 1994):

$$VPD_{\mathrm{a}} = SVP_{\mathrm{a}} - SVP_{\mathrm{d}} \quad \text{(A16)}$$

The saturated vapour pressure of the air (SVP_{a}) depends on T_{a} (Goudriaan and van Laar 1994):

$$SVP_{\mathrm{a}} = 610.7 * \exp[17.4 \times T_{\mathrm{a}}/(239 + T_{\mathrm{a}})]/1000 \quad \text{(A17)}$$

while the dew-point vapour pressure of the air (SVP_d) is related to dewpoint temperature, which is assumed as $T_{a,min}$, so SVP_d is given by:

$$SVP_{\mathrm{d}} = 610.7 * \exp[17.4 \times T_{\min}/(239 + T_{\min})]/1000 \quad \text{(A18)}$$

Absorbed PAR by sunlit and shaded fractions of canopy

Absorbed irradiance is estimated using the sun-shade model developed in de Pury and Farquhar (1997). The model assumes that the canopy is a single layer with the total leaf area index (LAI, m^2 leaf m^{-2} ground) partitioned into sunlit and shaded fractions. The total amount of absorbed photosynthetic active radiation (PAR) for absorbed by each fraction depends on direct and diffuse PAR above the canopy, leaf area index of the whole canopy, angle of solar elevation and leaf angle and transmissivity of PAR in the canopy.

Leaf area of the sunlit and shaded fractions, not explicitly used in this section, but in later sections, are given by de Pury and Farquhar (1997):

$$LAI_{\mathrm{sun}} = [1 - \exp(-k_{\mathrm{b}} LAI_{\mathrm{can}})]/k_{\mathrm{b}} \quad \text{(A19)}$$

$$LAI_{\mathrm{sh}} = LAI_{\mathrm{can}} - LAI_{\mathrm{sun}} \quad \text{(A20)}$$

In a previous section, I_{dir} and I_{dif} were calculated (A2 and A1, respectively). These are converted to photosynthetic photon flux density (PPFD, μmol photon m^{-2} s^{-1}) by assuming that the fraction of PAR to solar radiation above the canopy is 50% and that the ratio of quantum content and energy of direct and diffuse PAR are 4.56 and 4.25 μmol per J of PAR, respectively (Monteith and Unsworth 2013). So PPFD in I_{dir} and I_{dif} are calculated by:

$$I_{\mathrm{dir\_PAR}} = I_{\mathrm{dir}} \times 0.5 \times 4.56 \times 1000000 \quad \text{(A21)}$$

$$I_{\mathrm{dif\_PAR}} = I_{\mathrm{dif}} \times 0.5 \times 4.25 \times 1000000 \quad \text{(A22)}$$

Absorbed PAR by the canopy ($I_{abs,can}$, μmol PAR m^{-2} s^{-1}) is given by de Pury and Farquhar 1997:

$$I_{\mathrm{abs,can}} = (1 - \rho_{\mathrm{cb}}) I_{\mathrm{dir\_PAR}} [1 - \exp(-k'_{\mathrm{b}} LAI_{\mathrm{can}})] + (1 - \rho_{\mathrm{cd}}) I_{\mathrm{dif\_PAR}} [1 - \exp(-k'_{\mathrm{d}} LAI_{\mathrm{can}})] \quad \text{(A23)}$$

where ρ_{cb} and ρ_{cd} are the canopy-level reflection coefficient for direct and diffuse PAR [ρ_{cd} = 0.057; Leuning *et al.* (1995); de Pury and Farquhar (1997)], I_{dir_PAR} and I_{dif_PAR} (μmol photon m^{-2} s^{-1}) are direct and diffuse PAR at the top of the canopy, k'_b is direct and scattered direct

PAR extinction coefficient, k'_{d} is diffuse and scattered diffuse PAR extinction coefficient, LAI_{can} is the total LAI of the canopy.

The direct and scattered direct PAR extinction coefficient k'_{b} is given by:

$$k'_{\mathrm{b}} = k_{\mathrm{b}}\sqrt{1-\sigma} \tag{A24}$$

where k_{b} is the direct radiation extinction coefficient of the canopy, σ is the leaf-level scattering coefficient for PAR [= 0.2; Leuning *et al.* (1995); de Pury and Farquhar (1997)]. The direct radiation extinction coefficient of the canopy k_{b} is given by:

$$k_{\mathrm{b}} = G/\sin\{\alpha\} \tag{A25}$$

where α (radians) is the sun angle and G is the leaf shadow projection coefficient. If the spherical leaf-angle distribution (de Wit *et al.* 1978) is assumed, for a wide range of leaf and sun angles, G is approximated by 0.5 (Goudriaan 1988; Sinclair and Horie 1989; de Pury and Farquhar 1997). k_b is then given by:

$$k_{\mathrm{b}} = 0.5/\sin(\alpha) \tag{A26}$$

However, G can be derived more precisely from leaf and sun angles (Duncan *et al.* 1967):

$$G = \begin{cases} \cos\alpha\sin\beta\,, & \alpha \le \beta \\ \frac{2}{\pi}\sin\alpha\cos\beta\sin\theta + \left(1-\frac{\theta^{\circ}}{90}\right)\cos\alpha\sin\beta\,, & \alpha > \beta \end{cases} \tag{A27}$$

where β (radians) is the canopy-average leaf inclination relative to the horizontal and θ ($\theta°$ is θ in degrees) can be calculated from

$$\cos\theta = \cot\alpha\sin\beta \tag{A28}$$

The canopy-level reflection coefficient for direct PAR (ρ_{cb}) is given by:

$$\rho_{\mathrm{cb}} = 1 - \exp[2\rho_{\mathrm{h}}k_{\mathrm{b}}/(1+k_{\mathrm{b}})] \tag{A29}$$

where ρ_{h} is the reflection coefficient of the canopy with horizontal leaves and is given by:

$$\rho_h = \frac{1-(1-\sigma)^{1/2}}{1+(1-\sigma)^{1/2}} \tag{A30}$$

Absorbed PAR by the sunlit fraction of the canopy is given by the sum of direct, diffuse and the scattered components:

$$I_{\mathrm{abs,sun}} = (1-\sigma)I_{\mathrm{dir\_PAR}}[1-\exp(-k_{\mathrm{b}}LAI_{\mathrm{can}})]$$

$$+(1-\rho_{\mathrm{cd}})I_{\mathrm{dif\_PAR}}[1-\exp(-(k'_{\mathrm{d}}+k_{\mathrm{b}})LAI_{\mathrm{can}})]\frac{k'_{\mathrm{d}}}{k'_{\mathrm{d}}+k_{\mathrm{b}}}+$$

$$I_{\mathrm{dir\_PAR}}\left\{\begin{array}{c}(1-\rho_{\mathrm{cb}})[1-\exp(-(k'_{\mathrm{b}}+k_{\mathrm{b}})LAI_{\mathrm{can}})]\frac{k'_{\mathrm{b}}}{k'_{\mathrm{b}}+k_{\mathrm{b}}}\\ -(1-\sigma)[1-\exp(-2k_{\mathrm{b}}LAI_{\mathrm{can}})]\frac{1}{2}\end{array}\right\} \quad \text{(A31)}$$

Absorbed PAR by the shaded fraction of the canopy can be calculated by subtracting A31 from A23:

$$I_{\mathrm{abs,sh}} = I_{\mathrm{abs,can}} - I_{\mathrm{abs,sun}} \quad \text{(A32)}$$

Canopy specific leaf nitrogen profile

The profile of specific leaf nitrogen in the canopy is parameterised by specific leaf nitrogen averaged over canopy (SLN_{av}, g N m^{-2} leaf) and SLN at the top layer of the canopy (SLN_{o}), which is given by:

$$SLN_{\mathrm{o}} = SLN_{\mathrm{ratio\_top}} \times SLN_{\mathrm{av}} \quad \text{(A33)}$$

where $SLN_{\mathrm{ratio\_top}}$ is the ratio of SLN_{o} to SLN_{av}.

However, to adapt the SLN profile for V_{cmax}, J_{max} and R_{d} estimation for sunlit and shade leaf fractions using the approach in de Pury and Farquhar (1997), the SLN profile was expressed by de Pury and Farquhar (1997):

$$N(L) = (N_{\mathrm{o}} - N_{\mathrm{b}})\exp(-k_{\mathrm{n}}\,L/LAI_{\mathrm{can}}) + N_{\mathrm{b}} \quad \text{(A34)}$$

where L is the cumulative leaf area index (LAI, m^{-2} leaf m^{-2} ground) from top of canopy, N_{o} is SLN_{o} in mmol N m^{-2} leaf, N_{b} is the minimum value of N at or below which CO_2 assimilation rate is zero (= 25 mmol N m^{-2} for wheat (de Pury and Farquhar 1997); = 14 mmol N m^{-2} for maize (Sinclair and Horie 1989)), k_{n} is the coefficient of N allocation in the canopy. Total canopy nitrogen content (N_{c}) can be calculated by taking the definite integral of Eqn A34 between $L = LAI_{\mathrm{can}}$ and 0 (de Pury and Farquhar 1997):

$$N_{\mathrm{c}} = LAI_{\mathrm{can}}\{(N_{\mathrm{o}} - N_{\mathrm{b}})[1-\exp(-k_{\mathrm{n}})]/k_{\mathrm{n}} + N_{\mathrm{b}}\} \quad \text{(A35)}$$

The parameter k_{n} can be expressed in terms of SLN_{av} and $SLN_{\mathrm{ratio\_top}}$ by substituting Eqn A33 (SLN_{av} and SLN_{o} expressed in mmol N m^{-2} leaf by multiplying by 1000/14) into A34 and rearrange for k_{n}:

$$k_{\mathrm{n}} = -2\ln\left(\frac{N_{\mathrm{av}}-N_{\mathrm{b}}}{N_{\mathrm{o}}-N_{\mathrm{b}}}\right) \quad \text{(A36)}$$

Dependence of V_{cmax}, J_{max}, R_d and V_{pmax} on specific leaf nitrogen

V_{cmax}, J_{max} and R_d (whole canopy values) are calculated as follows. Their values (per leaf area) at the reference temperature (i.e. 25°C) are assumed to be linearly correlated with specific leaf nitrogen [e.g. Evans (1983) and Harley *et al.* (1992)], which can be modelled by de Pury and Farquhar (1997):

$$V_{\mathrm{cmax,l25}} = \chi_{\mathrm{Vc}}(N - N_{\mathrm{b}}) \tag{A37}$$

$$J_{\mathrm{max,l25}} = \chi_{\mathrm{J}}(N - N_{\mathrm{b}}) \tag{A38}$$

$$R_{\mathrm{d,l25}} = \chi_{\mathrm{Rd}}(N - N_{\mathrm{b}}) \tag{A39}$$

$$V_{\mathrm{pmax,l25}} = \chi_{\mathrm{Vp}}(N - N_{\mathrm{b}}) \tag{A40}$$

where $V_{cmax,l25}$, $J_{max,l25}$, $R_{d,l25}$ and $V_{pmax,l25}$ are V_{cmax25}, J_{max25}, R_{d25} and V_{pmax25} on a per leave area basis at the reference temperature. N is SLN expressed in g N m^{-2} leaf, χ_{Vc}, χ_{J}, χ_{Rd} and χ_{Vp} are the slope of the linear correlation between $V_{cmax,l25}$, $J_{max,l25}$, $R_{d,l25}$, $V_{pmax,l25}$ and N, respectively. $R_{d,l25}$ is assumed as $0.01V_{cmax,l25}$ for C_3 wheat (de Pury and Farquhar 1997) and 0 for C_4 maize (Massad *et al.* 2007), which can be implemented with $\chi_{\mathrm{R}} = 0.01\chi_{\mathrm{V}}$ and $\chi_{\mathrm{R}} = 0$, respectively. $V_{cmax,l25}$, $J_{max,l25}$, $R_{d,l25}$ and $V_{pmax,l25}$ are integrated over the whole canopy by de Pury and Farquhar (1997):

$$P_{\mathrm{can25}} = LAI_{\mathrm{can}}\chi_{\mathrm{P}}(N_{\mathrm{o}} - N_{\mathrm{b}})\frac{[1-\exp(-k_{\mathrm{n}})]}{k_{\mathrm{n}}} \tag{A41}$$

where P_{can25} is the value of parameters at 25ºC for the whole canopy, k_n is obtained from Eqn A36. Partitioning the parameters to sunlit and shaded fractions is achieved following the approach in de Pury and Farquhar (1997). Parameter for the sunlit fraction (P_{sun25}) at 25°C is given by:

$$P_{\mathrm{sun25}} = LAI_{\mathrm{can}}\chi_{\mathrm{P}}(N_{\mathrm{o}} - N_{\mathrm{b}}) \times \frac{[1-\exp(-k_{\mathrm{n}}-k_{\mathrm{b}}LAI_{\mathrm{can}})]}{k_{\mathrm{n}}+k_{\mathrm{b}}LAI_{\mathrm{can}}} \tag{A42}$$

and that of the shaded fraction (P_{sh25}) is given by the difference between the whole canopy and the sunlit fraction:

$$P_{\mathrm{sh25}} = P_{\mathrm{can25}} - P_{\mathrm{sun25}} \tag{A43}$$

Responses of P_{sun25} and P_{sh25} to leaf temperature (T_l) are modelled by Eqns 1 (for calculating V_{cmax}, R_d and V_{pmax}) and 2 (for calculating J_{max}) using parameters in Table S2.

Dependence of electron transport rate on absorbed PAR

A relationship between the electron transport rate of either the sunlit or shaded fractions (J_ε, where ε = sun or sh for indicating either the sunlit or shaded fraction) and absorbed PAR is required to define J_ε. At present, the relationship is empirical and the most frequently used expression is a non-rectangular hyperbola function (Farquhar and Wong 1984):

$$\theta J_\varepsilon^2 - J_\varepsilon\left(I_{2,\varepsilon} + J_{\max,\varepsilon}\right) + I_{2,\varepsilon}J_{\max,\varepsilon} = 0 \qquad \text{(A44)}$$

where I_2 is the PPFD on Photosystem II, $J_{\max}$ is the maximum electron transport rate (see Eqn A41 to A43 for calculations) and θ is an empirical curvature factor [~0.7; von Caemmerer (2013)] and assumed to be the same for both fractions). I_2 is calculated form absorbed PAR (I_{abs}) by either sunlit or shaded leaves by:

$$I_{2,\varepsilon} = I_{\mathrm{abs},\varepsilon} \times (1 - f)/2 \qquad \text{(A45)}$$

where $I_{abs,\varepsilon}$ is either I_{abs_sun} (Eqn A31) or I_{abs_sh} (Eqn A32), f is the spectral correction factor [~0.15 (Evans 1987) and assumed to be the same for both fractions]. The 2 is in the denominator as we assume $I_{abs,\varepsilon}$ is partitioned evenly to both Photosystem II and I (von Caemmerer 2000). Eqn A44 can be solved for J_ε as follows:

$$J_\varepsilon = \frac{I_{2,\varepsilon} + J_{\max,\varepsilon} - \sqrt{\left(I_{2,\varepsilon} + J_{\max,\varepsilon}\right)^2 - 4\theta J_{\max,\varepsilon} I_{2,\varepsilon}}}{2\theta} \qquad \text{(A46)}$$

Diffusion of CO_2 in the surrounding air into chloroplasts

In order for CO_2 in the surrounding air (C_a, μbar) to reach inside chloroplasts, we assume C_a has to diffuse through the leaf boundary-layer to reach leaf surface (C_s), diffuse through the stomata to reach the intercellular air space (C_i) and diffuse through the mesophyll component to reach inside chloroplasts (C_c). Diffusion of CO_2 through a component is determined by the conductance of the component. Leaf boundary-layer and stomatal conductance are considered in this model based on the leaf transpiration model described in Goudriaan and van Laar (1994); the importance of mesophyll conductance has been recently reviewed (Flexas *et al.* 2008). Chloroplastic CO_2 partial pressure for the sunlit and shaded fractions can be estimated based on Fick's first law of diffusion:

$$C_{\mathrm{c},\varepsilon} = C_\mathrm{a} - \frac{A_\varepsilon}{g_{\mathrm{b},\varepsilon}} - \frac{A_\varepsilon}{g_{\mathrm{s},\varepsilon}} - \frac{A_\varepsilon}{g_{\mathrm{m},\varepsilon}} \qquad \text{(A47)}$$

where g_b, g_s and g_m are leaf boundary, stomatal and mesophyll conductance for CO_2, respectively (these conductances have units of mol m^{-2} ground s^{-1}) and A is CO_2 assimilation. ε = sun or sh for indicating either the sunlit or shaded fraction. The conductance units are per ground area basis because they are the integrated value over the LAI of the fractions (Eqns A19 and A20), i.e.:

$$g_{\omega,\varepsilon} = g_{\omega,\mathrm{l}} \times LAI_{\varepsilon} \quad \text{(A48)}$$

where ω = either b, s or m to indicate either leaf boundary-layer, stomatal or mesophyll conductance, respectively.

However, $C_{i,\varepsilon}$ can be more simply estimated by using a C_i to C_a ratio (C_i/C_a), which has been found to remain consistent with respect to changes in C_a and a wide range of irradiance (Wong *et al.* 1979). This bypasses the need to quantify $g_{b,\varepsilon}$ and $g_{s,\varepsilon}$. $C_{c,\varepsilon}$ is then estimated by:

$$C_{c,\varepsilon} = C_i/C_a \times C_a - \frac{A_\varepsilon}{g_{m,\varepsilon}} \quad \text{(A49)}$$

where the C_i/C_a ratio is assumed to be the same for both fractions, but can change with VPD given by the correlation in Eqn 3 in the main text.

C_3 photosynthesis model

Net CO_2 assimilation rate (A, μmol CO_2 m^{-2} s^{-1}) of the sunlit or shaded fractions in the canopy can be given by Farquhar *et al.* (1980) and von Caemmerer (2000), assuming no triose phosphate utilisation limitation:

$$A_\varepsilon = \min\{A_{c,\varepsilon}, A_{i,\varepsilon}\} \quad \text{(A50)}$$

where ε = sun or sh for indicating either the sunlit or shade leaf fraction, A is given by the minimum RuBP-saturated (or Rubisco-limited) (A_c) or RuBP-regeneration-limited (or electron-transport-limited) (A_j) net CO_2 assimilation rate. For convenience, the subscription ε, used to indicate either the sunlit or shaded fraction, will be omitted in the rest of this and the subsequent sections.

RuBP-saturated (or Rubisco-limited) A (A_c) is given by Farquhar *et al.* (1980):

$$A_c = \frac{(C_c - \Gamma^*)V_{cmax}}{C_c + K_c(1 + O_c/K_o)} - R_d \quad \text{(A51)}$$

where C_c (μbar) is the chloroplastic CO_2 partial pressure, R_d (μmol m^{-2} s^{-1}) is the day respiration of leaves, Γ_* (μbar) is the CO_2 compensation point in the absence of R_d, V_{cmax} (μmol m^{-2} s^{-1}) is the maximum rate of Rubisco carboxylation (values for sunlit and shaded fraction can be calculated by Eqn A41 to A43), K_c and K_o are the Michaelis Menten constants of Rubisco carboxylation and oxygenation and have a unit of μbar, O_c is the chloroplastic O_2 partial pressure and is assumed to equal to the oxygen partial pressure measured in C_3 leaves (= 210000 μbar,).

The CO_2 compensation point in the absence of R_d, Γ_*, is given by:

$$\Gamma_* = \gamma_* O_c \quad \text{(A52)}$$

where γ_* is half the reciprocal of the relative CO_2/O_2 specificity of Rubisco, $S_{c/o}$. $S_{c/o}$ is given by:

$$S_{c/o} = \frac{K_o}{K_c}\frac{V_{cmax}}{V_{omax}} \quad \text{(A53)}$$

where V_{cmax}/V_{omax} is the maximum rate of Rubisco carboxylation over the maximum rate of Rubisco oxygenation.

RuBP-regeneration-limited (or electron-transport-limited) A (A_j), assuming NADPH-limited electron transport rate (Farquhar *et al.* 1980), is given by:

$$A_j = \frac{(C_c - \Gamma^*)J}{4C_c + 8\Gamma^*} - R_d \quad \text{(A54)}$$

where J (μmol m^{-2} s^{-1}) is the electron transport rate.

C_4 photosynthesis model

Enzyme-limited C_4 photosynthesis is given by von Caemmerer (2000):

$$A_c = \frac{(C_s - \gamma_* O_s)V_{cmax}}{C_s + K_c(1 + O_s/K_o)} - R_d \quad \text{(A55)}$$

where C_s is the bundle-sheath CO_2 partial pressure, γ_* is half of the reciprocal of $S_{c/o}$ (Eqn A53), O_c is the chloroplastic O_2 partial pressure. Other parameters are the same as those defined for the C_3 photosynthesis model and can also be found in Table S1.

Bundle-sheath O_2 partial pressure is given by Berry and Farquhar (1978):

$$O_s = \frac{\alpha A}{0.047 g_{bs}} + O_m \quad \text{(A56)}$$

where α is the fraction of PSII activity in the bundle sheath, which can range from 0 to 1 (von Caemmerer 2000) and is taken as 0.1 (Yin and Struik 2009), g_{bs} is bundle-sheath conductance (with units of mol m^{-2} ground s^{-1} bar^{-1}, whereas $g_{bs,l}$ has units of mol m^{-2} leaf s^{-1} bar^{-1}) for CO_2, O_m is mesophyll O_2 partial pressure and is assumed to equal to the oxygen partial pressure measured in C_3 leaves (= 210000 μbar).

The bundle-sheath CO_2 partial pressure is given by:

$$C_s = C_m + \frac{V_p - A_c - R_m}{g_{bs}} \quad \text{(A57)}$$

where C_m is the mesophyll CO_2 partial pressure, V_p is the rate of phosphoenolpyruvate (PEP) carboxylation, R_m is mesophyll mitochondrial respiration.

The rate of PEP carboxylation is given by:

$$V_p = \min\left\{\frac{C_m V_{pmax}}{C_m + K_p}, V_{pr}\right\} \quad \text{(A58)}$$

where V_{pmax} is the maximum PEP carboxylase activity, K_p is the Michaelis-Menten constant of PEP carboxylase for CO_2 and V_{pr} is the PEP regeneration rate. The left term in the argument occurs when CO_2 is limiting PEP carboxylation rate, while the right term occurs when the rate of PEP regeneration is limiting.

Light- and electron-transport-limited C_4 photosynthesis is given by von Caemmerer (2000):

$$A_j = \frac{(1 - \gamma_* O_s/C_s)(1 - x)J_t}{3(1 + 7\gamma_* O_s/(3C_s))} - R_d \quad \text{(A59)}$$

where x is the fraction of electron transport partitioned to mesophyll chloroplasts, J_t is the total electron transport rate from both the mesophyll and bundle-sheath cells, which can be calculated by Eqn A46 (von Caemmerer 2000), assuming J_t and J are synonymous.

The bundle-sheath CO_2 partial pressure is given by:

$$C_s = C_m + \frac{xJ_t/2 - A_j - R_m}{g_{bs}} \quad \text{(A60)}$$

Couple photosynthesis with CO_2 diffusion model

Analytical solution of C_3 photosynthesis model coupled with the CO_2 diffusion model can be obtained by combining Eqn A49 and A51 for A_c calculation; and combining Eqn A49 and A54 for A_j calculation and solving for A. Remember these are done for both sunlit and shaded fractions of the canopy. The resulting analytical solution is:

$$A = \left(-\sqrt{a^2 - 4b} + c\right)/2d \quad \text{(A61)}$$

where a, b, c and d are lumped coefficients as follows.

$$a = -x_a C_a g_m - g_m x_2 + R_d - x_1 \quad \text{(A62)}$$

$$b = -x_a C_a g_m R_d + x_a C_a g_m x_1 - g_m R_d x_2 - g_m \Gamma_* x_1 \quad \text{(A63)}$$

$$c = x_a C_a g_m + g_m x_2 - R_d + x_1 \quad \text{(A64)}$$

$$d = 1 \quad \text{(A65)}$$

where x_1 and x_2 are lumped coefficients and are given in the following table.

Table A3.

	x_1	x_2
A_c	V_{cmax}	$K_c(1+O_c/K_o)$
A_j	$J/4$	$2\Gamma_*$

Once A_c or A_j are calculated, C_c can be back calculated by Eqn A49 and reported.

An analytical solution of the C_4 photosynthesis model coupled with the CO_2 diffusion model can be obtained by combining Eqn A49, A55, A56 and A57 for A_c calculation; and combing Eqn A49, A56, A59 and A60 for A_j calculation. An approximation is made to allow analytical solution of A_c (Eqn A55) when the left element in the argument in Eqn A58 applies:

$$\frac{C_m V_{pmax}}{C'_m + K_p} \approx \Delta C_m \quad \text{(A66)}$$

where Δ is the slope of a line from the origin to a point on the Michaelis-Menten curve (described by the left-hand side of Eqn A66) at an arbitrary C_m, C'_m, and is given by:

$$\Delta = V_{pmax}/\left(C'_m + K_p\right) \quad \text{(A67)}$$

Sufficiently accurate calculation of A_c (within ± 1%), when Eqn A66 is applied, can be obtained by optimising C'_m in Eqn A67, involving just three iterative calculations. In the first iterative step, C'_m is set to 160, the resulting calculated C_m (Eqn A49) is input into A67 for the second iterative step, and repeated again for a third time. Testing with C_a between 400 and 1200 µbar show A_c converged to within ± 1% of the fully optimised value with this optimisation procedure.

The lumped coefficients in Eqn A61 with the C_4 photosynthesis model are as follows.

$$a = -0.047xC_a g_m g_{bs} - 0.047xC_a g_m x_4 - \alpha g_m R_d x_2 - \alpha g_m \gamma_* x_1 - 0.047O_m g_m g_{bs} x_2 - 0.047g_m g_{bs} x_3 + 0.047g_m R_m + 0.047g_m R_d - 0.047g_m x_1 - 0.047g_m x_5 + 0.047g_{bs} R_d - 0.047g_{bs} x_1 + 0.047R_d x_4 - 0.047x_1 x_4 \quad \text{(A68)}$$

$$b = (-\alpha g_m x_2 + 0.047g_m + 0.047g_{bs} + 0.047x_4)[-0.047xC_a g_m g_{bs} R_d + 0.047xC_a g_m g_{bs} x_1 - 0.047xC_a g_m R_d x_4 + 0.047xC_a g_m x_1 x_4 - 0.047O_m g_m g_{bs} R_d x_2 - 0.047g_m g_{bs} R_d x_3 - 0.047O_m g_m g_{bs} \gamma_* x_1 + 0.047g_m R_m - 0.047g_m R_m x_1 - 0.047g_m R_d x_5 + 0.047g_m x_1 x_5] \quad \text{(A69)}$$

$c = 0.047xC_a g_m g_{bs} + 0.047xC_a g_m x_4 + \alpha g_m R_d x_2 + \alpha g_m \gamma_* x_1 + 0.047O_m g_m g_{bs} x_2 + 0.047g_m g_{bs} x_3 - 0.047g_m R_m - 0.047g_m R_d + 0.047g_m x_1 + 0.047g_m x_5 - 0.047g_{bs} R_d + 0.047g_{bs} x_1 - 0.047R_d x_4 + 0.047x_1 x_4$ (A70)

$d = -\alpha g_m x_2 + 0.047g_m + 0.047g_{bs} + 0.047x_4$ (A71)

where x_1 through to x_5 are lumped coefficients and are given in the following table.

Table S4.

	x_1	x_2	x_3	x_4	x_5
A_c (PEP-saturated rate)	V_{cmax}	K_c/K_o	K_c	Δ (Eqn A67)	0
A_c (PEP-regeneration-limited rate)				0	V_{pr}
A_j	$(1 - x)J_t/3$	$7/3\gamma_*$	0	0	$xJ_t/2$

Once A_c or A_j are calculated using the analytical solutions, O_s, C_m, V_p, C_s, and φ can be back calculated and reported. O_s and C_m, can be back calculated by Eqns A56 and A49, respective. In the case of A_c, V_p can be back calculated by the expression $x_4C_m + x_5$ for either the PEP-saturated or PEP-regeneration-limited rate (Table S4); for A_j, the same expression applies, but the corresponding parameter is no longer called V_p. C_s can be back calculated by Eqns A57 and A60 for A_c and A_j, respectively. φ is back calculated for A_c by Farquhar (1983):

$\phi = g_{\mathrm{bs}}(C_{\mathrm{s}} - C_{\mathrm{m}})/V_{\mathrm{p}}$ (A72)

Diurnal canopy photosynthesis and daily above-ground canopy (shoot) biomass increment

Diurnal canopy photosynthesis ($A_{can,DAY}$) is calculated by summing the calculated A (Eqn A50) of the sunlit and shaded fractions of the canopy at the start of the i^{th} hour ($A_{can,inst,i}$), integrating hourly by multiplying by 3600 and summing over a diurnal period:

$A_{\mathrm{can,DAY}} = \sum_{i=\lceil t_{\mathrm{sunrise}} \rceil}^{\lfloor t_{\mathrm{sunset}} \rfloor} \left(A_{\mathrm{can,inst},i} \times 3600 \right)$ (A73)

the subscript DAY is used despite this being a diurnal calculation as photosynthesis only occurs in the diurnal period, but it represents the assimilated CO_2 over a day. $\lceil t_{\mathrm{sunrise}} \rceil$ is the ceiling function applied to $t_{sunrise}$ (giving the first whole hour after $t_{sunrise}$) and $\lfloor t_{\mathrm{sunset}} \rfloor$ is the floor function applied to t_{sunset} (giving the whole hour just before t_{sunset}). The reason for this set up is that $t_{sunrise}$ and t_{sunset} (Eqns A13 and A14, respectively) vary with *LAT* and *DAY*. The calculated $A_{can,DAY}$ represents the gross carbon gain for *DAY*.

To calculate daily above-ground canopy biomass increment ($BIO_{shoot,DAY}$, g biomass day^{-1}) firstly, a conversion ratio (B, g biomass g^{-1} CO_2) was assumed to convert $A_{can,DAY}$ to daily whole-plant biomass increment ($BIO_{total,DAY}$, g biomass day^{-1}). The conversion ratio combined factors allowing for biochemical conversion of CO_2 to biomass and CO_2 loss due to maintenance respiration (Sinclair and Horie 1989), which is consistent with the conservative respiration:photosynthesis ratio approach (Gifford 2003). Secondly, the fraction of $BIO_{total,DAY}$ partitioned to shoot is given by P_{shoot}, which is the fraction of above-ground (shoot) biomass to the total (shoot + root). Therefore, $BIO_{shoot,DAY}$ is calculated as:

$$\mathrm{BIO}_{\mathrm{shoot,DAY}} = A_{\mathrm{can,DAY}} \times B \times P_{\mathrm{shoot}} \tag{A74}$$

where B is taken as 0.41 g biomass (g CO_2)$^{-1}$ for cereal crops such as rice and maize (Sinclair and Horie 1989) and P_{shoot} is stage dependent (https://www.apsim.info/Portals/0/Documentation/Crops/WheatDocumentation.pdf).

Daily canopy radiation use efficiency and extinction coefficient

Radiation use efficiency on a daily basis (RUE_{DAY}, g biomass MJ^{-1}) is calculated as the ratio of $BIO_{shoot,DAY}$ to total solar radiation intercepted by the canopy (RAD_{DAY}, MJ m^{-2} ground day^{-1}) on *DAY*.

$$\mathrm{RUE}_{\mathrm{DAY}} = \mathrm{BIO}_{\mathrm{shoot,DAY}}/\mathrm{RAD}_{\mathrm{DAY}} \tag{A75}$$

Where RAD_{DAY} is given by:

$$\mathrm{RAD}_{\mathrm{DAY}} = \sum_{\lceil t_{\mathrm{sunrise}} \rceil}^{\lfloor t_{\mathrm{sunset}} \rfloor} \left(I_{\mathrm{o},i} \times F_{\mathrm{can},i} \times 3600 \right) \tag{A76}$$

where $I_{o,i}$ is defined by Eqn A3 at the i^{th} hour and $F_{can,i}$ is the proportion of solar radiation intercepted by the canopy at the i^{th} hour given by:

$$F_{\mathrm{can},i} = 1 - \exp\left(-LAI_{\mathrm{can}} \times k_{\mathrm{b},i}\right) \tag{A77}$$

where k_b is defined by Eqn A25.

Canopy radiation extinction coefficient on a daily basis (k_{DAY}) is given by:

$$k_{\mathrm{DAY}} = -\ln\left(1 - \frac{\mathrm{RAD}_{\mathrm{DAY}}}{S_{\mathrm{g}}}\right)/LAI_{\mathrm{can}} \tag{A78}$$

which depends on the ratio of intercepted solar radiation by the canopy solar radiation reaching the ground, S_g (Eqn A4).

Appendix 2: List of symbols

Table S1. Description of symbols used in the Diurnal Canopy Photosynthesis Simulator (DCaPS).

Symbol	Description	Units	Note	Value and reference	Equation
Daily Canopy Summary					
$A_{\mathrm{can,inst}}$	Instantaneous canopy CO_2 assimilation	μmol CO_2 m^{-2} ground s^{-1}			A73
$A_{\mathrm{can,DAY}}$	Diurnal canopy CO_2 assimilation	μmol CO_2 m^{-2} ground day^{-1}			A73
B	Conversion ratio combines factors allowing for biochemical conversion and maintenance respiration	g biomass (g CO_2)$^{-1}$	A	0.41 (wheat and sorghum) (Sinclair and Horie 1989)	A74
$BIO_{\mathrm{total,DAY}}$	Daily total biomass increment	g biomass m^{-2} ground day^{-1}			A74
P_{shoot}	Fraction of above-ground (shoot) biomass to the total (shoot + root)	g shoot biomass (g total biomass)$^{-1}$	A		A74
$\mathrm{BIO}_{\mathrm{shoot,DAY}}$	Daily above-ground canopy (shoot) biomass increment	g biomass m^{-2} ground day^{-1}	E		A74
k_{DAY}	Canopy solar radiation extinction coefficient on daily basis				A78
$\mathrm{RAD}_{\mathrm{DAY}}$	Total daily intercepted solar radiation	MJ m^{-2} ground day^{-1}			A76
$\mathrm{RUE}_{\mathrm{DAY}}$	Radiation use efficiency on daily basis	g biomass MJ^{-1}			A75
Environmental Parameters					
S_o	Total daily extra-terrestrial solar radiation	MJ m^{-2} ground day^{-1}			A5
S_g	Total daily incident solar radiation	MJ m^{-2} ground day^{-1}			A4
RATIO	Atmospheric transmission ratio		A,D		A4
sc	Solar constant	J m^{-2} ground s^{-1}	A	1360	A5
Lat	Latitude in radians (negative in the southern hemisphere)	radians	A		A5
$R\mathrm{l}$	Radius vector	radians			A6
$D\mathrm{l}$	Solar declination	radians			A8
$W\mathrm{l}°$	Sunset hour-angle	°			A7
$L\mathrm{l}$	Day length	hr			A10
DAY	Day of year		A,D		
t_{frac}	t as a fraction of $L\mathrm{l}$				A12
t_{sunrise}	Time of sunrise	hr			A13
t_{sunset}	Time of sunset	hr			A14
α_{sun}	Angle of solar elevation	radians or degree			A9
T_{a}	Air temperature	ºC			A15
$T_{\mathrm{a,max}}$	Maximum T_{a} of *DAY*	ºC	A,D		A15
$T_{\mathrm{a,min}}$	Minimum T_{a} of *DAY*	ºC	A,D		A15
m	Amount of time since time of minimum temperature	hr			A15
n	Amount of time since t_{sunset}	hr			A15
x_{lag}	Lag coefficient for the maximum temperature from t_{sunrise}		A	1.8 (Parton and Logan 1981)	A15
y_{lag}	Lag coefficient for the night-time temperature from t_{sunrise}		A	2.2 (Parton and Logan 1981)	A15

z_{lag}	Lag coefficient for the minimum temperature from $t_{sunrise}$		A	1 (parameterised with hourly temperature data at Gatton, Australia)	A15
VPD_a	Air vapour pressure deficit	kPa			A16
C_a	Air CO_2 partial pressure	μbar	A	400	
O_a	Air O_2 partial pressure	μbar	A	210000	
I_o	Total incident solar radiation	MJ m^{-2} ground s^{-1}			A3
I_{dir}	Incident direct radiation	MJ m^{-2} ground s^{-1}			A2
I_{dif}	Incident diffuse radiation	MJ m^{-2} ground s^{-1}			A1
I_{o_PAR}	Total incident photosynthetic active radiation	μmol PAR m^{-2} ground s^{-1}		$I_{dir,PAR} + I_{dif,PAR}$	
I_{dir_PAR}	Direct incident photosynthetic active radiation	μmol PAR m^{-2} ground s^{-1}			A21
I_{dif_PAR}	Diffuse incident photosynthetic active radiation	μmol PAR m^{-2} ground s^{-1}			A22
$I_{abs,can}$	Absorbed PAR by the canopy	μmol PAR m^{-2} ground s^{-1}			A23
$I_{abs,sun}$	Absorbed PAR by the sunlit fraction of the canopy	μmol PAR m^{-2} ground s^{-1}			A31
$I_{abs,sh}$	Absorbed PAR by the shaded fraction of the canopy	μmol PAR m^{-2} ground s^{-1}			A32
Canopy Attribute and Architecture Parameters					
LAI_{can}	Canopy leaf area index	m^2 leaf m^{-2} ground	A,D		A20
LAI_{sun}	LAI of the sunlit leaf fraction	m^2 leaf m^{-2} ground			A19
LAI_{sh}	LAI of the shade leaf fraction	m^2 leaf m^{-2} ground			A20
L	Cumulative LAI from the top of canopy	m^2 leaf m^{-2} ground			
k_b'	Direct and scattered direct PAR extinction coefficient				A24
k_d'	Diffuse and scattered diffuse PAR extinction coefficient				A24
k_b	Direct radiation extinction coefficient		D		A25
k_d	Diffuse PAR extinction coefficient		A	0.78 (de Pury and Farquhar 1997)	
σ	Leaf-level scattering coefficient for PAR		A	0.15 (de Pury and Farquhar 1997)	
ρ_{cb}	Canopy-level reflection coefficient for direct PAR				A29
ρ_{cd}	Canopy-level reflection coefficient for diffuse PAR		A	0.036 (de Pury and Farquhar 1997)	
G	Leaf shadow projection coefficient				A27
β	Canopy-average leaf inclination relative to the horizontal	radians	A	60° (spherical leaf angle distribution) (de Pury and Farquhar 1997)	A27
T_l	Leaf temperature	°C	A	T_a	1, 2

Canopy Nitrogen Status Parameters					
SLN_{av}	Specific leaf nitrogen averaged over the whole canopy	g N m^{-2} leaf	A,D	1.45 (wheat) (de Pury and Farquhar 1997), 1.36 (sorghum) (van Oosterom *et al.* 2010)	A33
SLN_{ratio_top}	Ratio of SLN_o to SLN_{av}	g N m^{-2} leaf	A,D	1.32 (wheat) (de Pury and Farquhar 1997), 1.30 (sorghum) (van Oosterom *et al.* 2010)	A33
SLN_o	SLN at the top of canopy	g N m^{-2} leaf			A33
$N(L)$	SLN at L	mmol N m^{-2} leaf			A34
N_o	SLN at the top of canopy	mmol N m^{-2} leaf			A33
N_b	Base SLN at or below which leaf photosynthesis = 0	mmol N m^{-2} leaf	A	25 (wheat) (de Pury and Farquhar 1997), 14 (sorghum) (Sinclair and Horie 1989)	A34
k_n	Coefficient of nitrogen allocation through canopy				A36
Photosynthesis Parameters					
χ_V	Slope of linear relationship between V_{max} per leaf are at 25°C and N	μmol CO_2 $mmol^{-1}$ N s^{-1}	B	1.16 (de Pury and Farquhar 1997) (wheat), 0.35 (sorghum) (Massad *et al.* 2007)	A37
χ_J	Slope of linear relationship between J_{max} per leaf are at 25°C and N	μmol CO_2 $mmol^{-1}$ N s^{-1}	B	2.4 (wheat) (de Pury and Farquhar 1997), 2.4 (sorghum) (Massad *et al.* 2007)	A38
χ_R	Slope of linear relationship between R_d per leaf are at 25°C and N	μmol CO_2 $mmol^{-1}$ N s^{-1}	B	$0.01\chi_V$ (wheat) (de Pury and Farquhar 1997), 0 (sorghum) (Massad *et al.* 2007)	A39
χ_P	Slope of linear relationship between V_{pmax} per leaf are at 25°C and N	μmol CO_2 $mmol^{-1}$ N s^{-1}	B,C_4	1.1 (sorghum) (Massad *et al.* 2007)	A40
V_{cmax}	Maximum rate of Rubisco carboxylation	μmol CO_2 m^{-2} ground s^{-1}		Table 2	
J_{max}	Maximum rate of electron transport	μmol CO_2 m^{-2} ground s^{-1}		Table 2	
R_d	Leaf day respiration	μmol CO_2 m^{-2} ground s^{-1}		Table 2	

R_m	Mesophyll mitochondrial respiration	μmol CO_2 m^{-2} ground s^{-1}	C_4	$0.5R_d$ (von Caemmerer 2000)	
K_c	Michaelis-Menten constant of Rubisco for CO_2	μbar		Table 2	
K_o	Michaelis-Menten constant of Rubisco for O_2	μbar		Table 2	
A_c	RuBP-saturated (or Rubisco-limited) net CO_2 assimilation rate	μmol m^{-2} ground s^{-1}			
A_j	RuBP-regeneration-limited (or electron-transport-limited) net CO_2 assimilation rate	μmol m^{-2} ground s^{-1}			
Γ_*	CO_2 compensation point in the absence of R_d	μbar			A52
γ_*	Half the reciprocal of $S_{c/o}$			$0.5/S_{c/o}$	
$S_{c/o}$	Relative CO_2/O_2 specificity of Rubisco	bar bar^{-1}			A53
V_{cmax}/V_{omax}	Ratio of maximum rate of Rubisco carboxylation to maximum rate of Rubisco oxygenation			Table 2	A53
J	Potential electron transport rate	μmol e^- m^{-2} ground s^{-1}			A46
θ	Empirical curvature factor		A	0.7 (de Pury and Farquhar 1997)	A46
f	Spectral correction factor		A	0.15 (de Pury and Farquhar 1997)	A46
I_2	PAR absorbed by Photosystem II	μmol PAR m^{-2} ground s^{-1}			A45
α	Fraction of PSII activity in the bundle sheath		C_4	0.1 (Yin and Struik 2009)	A56
V_p	Rate of PEP carboxylation	μmol CO_2 m^{-2} ground s^{-1}	C_4		A58
V_{pmax}	Maximum PEP carboxylase activity	μmol CO_2 m^{-2} ground s^{-1}	C_4	Table 2	
K_p	Michaelis-Menten constant of PEP carboxylase for CO_2	μbar	C_4	Table 2	
$V_{pr,l}$	PEP regeneration rate per leaf area	μmol CO_2 m^{-2} leaf s^{-1}	A,C_4	80 (von Caemmerer 2000)	
V_{pr}	PEP regeneration rate	μmol CO_2 m_{-2} ground s^{-1}	C_4		A58
J_t	Potential electron transport rate (symbol for C_4)	μmol e^- m^{-2} ground s^{-1}	C_4		A46
x	Fraction of electron transport partitioned to mesophyll chloroplasts		A,C_4	0.4 (von Caemmerer 2000)	A59
CO_2 Diffusion Parameters					
C_i	Intercellular airspace CO_2 partial pressure	μbar			
C_m	Mesophyll CO_2 partial pressure	μbar	C_4		A57, A60
C_c	Chloroplastic CO_2 partial pressure at the site of Rubisco carboxylation	μbar			A51, A54
C_s	Bundle-sheath CO_2 partial pressure	μbar	C_4		A55, A59
O_l	O_2 partial pressure inside C_3 and C_4 leaves	μbar		O_a	
O_c	Chloroplastic O_2 partial pressure at the site of Rubisco carboxylation	μbar		O_l	
O_m	Mesophyll O_2 partial pressure	μbar	C_4	O_l	A56
O_s	Bundle-sheath O_2 partial pressure	μbar	C_4		A56

a	Slope of linear relationship between C_i/C_a and VPD_a	kPa^{-1}		-0.12 (C_3), -0.19 (C_4) (Zhang and Nobel 1996)	3
b	Intercept of linear relationship between C_i/C_a and VPD_a			0.9 (C_3), 0.84 (C_4) (Zhang and Nobel 1996)	3
C_i/C_a	Ratio of C_i to C_a		A		3
g_m	Mesophyll conductance for CO_2	mol CO_2 m^{-2} ground s^{-1} bar^{-1}	B	Table 2	A47
g_{bs}	Bundle-sheath conductance for CO_2	mol CO_2 m^{-2} ground s^{-1} bar^{-1}	C_4	0.003 (von Caemmerer 2000)	A56

A: 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 S2. C_3 and C_4 temperature response parameters used in equations 1 ($P = P_{25}e^{(c-b/(T_l+273))}$) and 2 ($P = P_{25}e^{-\left(\frac{T_l-T_{opt}}{\Omega}\right)^2+\left(\frac{25-T_{opt}}{\Omega}\right)^2}$) in the main text

		C_3			C_4		
Parameter	**Units**	P_{25}	***c*** **(dimensionless)**	***b*** **(K)**	P_{25}	***c*** **(dimensionless)**	***b*** **(K)**
K_c	µbar	272.4[1]	32.7[1]	9741.4[1]	1210[4]	25.9[4]	7721.9[4]
K_o	µbar	165800[1]	9.6[1]	2853.0[1]	292000[4]	4.2[4]	1262.9[4]
V_{cmax}/V_{omax}	-	4.6[1]	13.2[1]	3945.7[1]	5.4[4]	9.1[4]	2719.5[4]
V_{cmax}	µmol m^{-2} s^{-1}	A	26.4[2]	7857.8[2]	A	31.5[4]	9381.8[4]
R_d	µmol m^{-2} s^{-1}	A	18.7[2]	5579.7[2]	-	-	-
K_p	µbar	-	-	-	139	14.6[4]	4366.1[4]
V_{pmax}	µmol m^{-2} s^{-1}	-	-	-	A	38.2[4]	11402.4[4]
		P_{25}	T_{opt} **(°C)**	***Ω*** **(K)**	P_{25}	T_{opt} **(°C)**	***Ω*** **(K)**
J_{max}	µmol m^{-2} s^{-1}	A	28.8[3]	15.5[3]	A	32.6[5]	15.3[5]
g_m	µmol m^{-2} s^{-1} bar^{-1}	0.55	34.3[1]	20.8[1]	0.55	34.3[1]	20.8[1]

A: variable. -: not applicable (see the main 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).

References

Bernacchi, CJ, Portis, AR, Nakano, H, von Caemmerer, S, Long, SP (2002) Temperature response of mesophyll conductance. Implications for the determination of Rubisco enzyme kinetics and for limitations to photosynthesis in vivo. *Plant Physiology* **130**, 1992-1998.

Bernacchi, CJ, Singsaas, EL, Pimentel, C, Portis Jr, AR, Long, SP (2001) Improved temperature response functions for models of Rubisco-limited photosynthesis. *Plant, Cell & Environment* **24**, 253-259.

Berry, J, Farquhar, G (1978) The CO2 concentrating function of C4 photosynthesis. A biochemical model. In 'Photosynthesis 77. Proceedings of the fourth international congress on photosynthesis. [Hall, D. O.; Coombs, J.; Goodwin, T. J. (Editors)].' pp. 119-131. (Biochemical Society of London: London)

Boyd, RA, Gandin, A, Cousins, AB (2015) Temperature response of C4 photosynthesis: Biochemical analysis of Rubisco, Phosphoenolpyruvate Carboxylase and Carbonic Anhydrase in Setaria viridis. *Plant Physiology*

Brock, TD (1981) Calculating solar-radiation for ecological-studies. *Ecological Modelling* **14**, 1-19.

Charles-Edwards, DA (Eds D Doley, GM Rimmington (1986) 'Modelling plant growth and development / by David A. Charles-Edwards, David Doley and Glynn M. Rimmington.' (Academic Press: Sydney)

Collares-Pereira, M, Rabl, A (1979) The average distribution of solar radiation-correlations between diffuse and hemispherical and between daily and hourly insolation values. *Solar Energy* **22**, 155-164.

de Pury, DGG, Farquhar, GD (1997) Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models. *Plant Cell and Environment* **20**, 537-557.

de Wit, CT, Goudriaan, J, van Laar, HH, Penning de Vries, FWT, Rabbinge, R, van Keulen, H, Sibma, L, de Jonge, C (1978) 'Simulation of assimilation, respiration and transpiration of crops.' (Pudco, Wageningen: Simulation Monographs)

Duncan, WG, Loomis, RS, Williams, WA, Hanau, R (1967) A model for simulating photosynthesis in plant communities. *Hilgardia* **38**, 181-&.

Evans, JR (1983) Nitrogen and Photosynthesis in the Flag Leaf of Wheat (Triticum aestivum L.). *Plant Physiology* **72**, 297-302.

Evans, JR (1987) The dependence of quantum yield on wavelength and growth irradiance. *Australian Journal of Plant Physiology* **14**, 69-79.

Farquhar, GD (1983) On the nature of carbon isotope discrimination in C4 species. *Australian Journal of Plant Physiology* **10**, 205-226.

Farquhar, GD, von Caemmerer, S, Berry, JA (1980) A biochemical model of photosynthetic CO2 assimilation in leaves of C3 species. *Planta* **149**, 78-90.

Farquhar, GD, Wong, SC (1984) An empirical-model of stomatal conductance. *Australian Journal of Plant Physiology* **11**, 191-209.

Flexas, J, Ribas-Carbo, M, Diaz-Espejo, A, Galmes, J, Medrano, H (2008) Mesophyll conductance to CO2: current knowledge and future prospects. *Plant Cell and Environment* **31**, 602-621.

Gifford, RM (2003) Plant respiration in productivity models: conceptualisation, representation and issues for global terrestrial carbon-cycle research. *Functional Plant Biology* **30**, 171-186.

Goudriaan, J (1988) The bare bones of leaf-angle distribution in radiation models for canopy photosynthesis and energy exchange. *Agricultural and Forest Meteorology* **43**, 155-169.

Goudriaan, J, van Laar, HH (1994) 'Modelling potential crop growth processes : textbook with exercises.' (Kluwer Academic Publishers: Dordrecht; Boston)
Hammer, GL, Wright, GC (1994) A theoretical-analysis of nitrogen and radiation effects on radiation use efficiency in peanut. *Australian Journal of Agricultural Research* **45**, 575-589.
Harley, PC, Loreto, F, Di Marco, G, Sharkey, TD (1992) Theoretical Considerations when Estimating the Mesophyll Conductance to CO(2) Flux by Analysis of the Response of Photosynthesis to CO(2). *Plant Physiology* **98**, 1429-1436.
Leuning, R, Kelliher, FM, De Pury, DGG, Schulze, ED (1995) Leaf nitrogen, photosynthesis, conductance and transpiration: scaling from leaves to canopies. *Plant, Cell & Environment* **18**, 1183-1200.
Massad, R-S, Tuzet, A, Bethenod, O (2007) The effect of temperature on C4-type leaf photosynthesis parameters. *Plant, Cell & Environment* **30**, 1191-1204.
Monteith, JL, Unsworth, MH (2013) Chapter 5 - Radiation Environment. In 'Principles of Environmental Physics (Fourth Edition).' (Eds JL Monteith, MH Unsworth.) pp. 49-79. (Academic Press: Boston)
Parton, WJ, Logan, JA (1981) A model for diurnal variation in soil and air temperature. *Agricultural Meteorology* **23**, 205-216.
Sinclair, TR, Horie, T (1989) Leaf nitrogen, photosynthesis, and crop radiation use efficiency - a review. *Crop Science* **29**, 90-98.
Spitters, CJT (1986) Separating the diffuse and direct component of global radiation and its implications for modeling canopy photosynthesis Part II. Calculation of canopy photosynthesis. *Agricultural and Forest Meteorology* **38**, 231-242.
van Oosterom, EJ, Borrell, AK, Chapman, SC, Broad, IJ, Hammer, GL (2010) Functional dynamics of the nitrogen balance of sorghum: I. N demand of vegetative plant parts. *Field Crops Research* **115**, 19-28.
von Caemmerer, S (2000) 'Biochemical models of leaf photosynthesis. Vol. 2.' (CSIRO Publishing: Collingwood, Australia)
von Caemmerer, S (2013) Steady-state models of photosynthesis. *Plant Cell and Environment* **36**, 1617-1630.
Wong, SC, Cowan, IR, Farquhar, GD (1979) Stomatal conductance correlates with photosynthetic capacity. *Nature* **282**, 424-426.
Yin, X, Struik, PC (2009) C-3 and C-4 photosynthesis models: An overview from the perspective of crop modelling. *Njas-Wageningen Journal of Life Sciences* **57**, 27-38.
Zhang, H, Nobel, P (1996) Dependency of Ci/Ca and Leaf Transpiration Efficiency on the Vapour Pressure Deficit. *Functional Plant Biology* **23**, 561-568.