Supplementary Material

1 Supplementary Data

The analytical solution proposed is valid when leaf surface CO_2 and humidity are known or assumed to be equal to the values in bulk air.

Description of the system of equations in a coupled photosynthesis-stomatal conductance model

Leaf photosynthesis sub-model

The biochemical model for C_3 photosynthesis proposed by Farquhar, von Caemmerer and Berry (1980) was used for computing the biochemical demand for leaf net CO_2 assimilation (A, µmol m^{-2} s^{-1}). According to the model, A is limited by the slowest of the following processes: (1) carboxylation rate limited by Ribulose biphosphate-carboxylase-oxygenase activity (Rubisco-limited, A_c, see Eqn 1), or (2) carboxylation rate limited by the rate of Ribulose 1-5 bisphosphate regeneration (RuBP-limited or electron transport limited, A_j, as described by Eqn 2). A third possible limitation by triose phosphate at high CO_2 (Farquhar et al., 1980) may also be considered (Eqn 3).

$$A_c = V_{cmax} \frac{\left(C_c - \Gamma^*\right)}{C_c + K_c\left(1 + O_i / K_o\right)} - R_d \qquad (1)$$

$$A_j = \frac{J\left(C_c - \Gamma^*\right)}{4\left(C_c + 2\Gamma^*\right)} - R_d \qquad (2)$$

$A_e = 0.5\ V_{cmax}$ (As defined in JULES for C_3 species, Clark et al., 2011) (3)

where R_d (µmol m^{-2} s^{-1}) is the leaf respiration in the light or day respiration, Γ^* (Pa) is the chloroplastic CO_2 photocompensation point in the absence of mitochondrial respiration, C_c (Pa) is the chloroplastic CO_2 concentration, and K_c (Pa) and K_o (Pa) are the Michaelis-Menten constants for carboxylation and oxygenation, respectively. O_i (Pa) is the leaf internal oxygen concentration (assumed equal to that of the external air), V_{cmax} (µmol m^{-2} s^{-1}) is the maximum carboxylation rate and J (µmol m^{-2} s^{-1}) is the electron transport rate. J depends on the maximum photosynhtetic electron transport rate (J_{max}, µmol m^{-2} s^{-1}) and photosynthetic quantum flux density (PPFD, µmol m^{-2} s^{-1}) and was computed according to a non-rectangular hyperbola (Farquhar and Wong, 1984):

$$J = \frac{\alpha PPFD + J_{max} - \sqrt{(\alpha PPFD + J_{max})^2 - 4\alpha\delta PPFD J_{max}}}{2\delta} \qquad (4)$$

where α is the initial quantum yield and δ is the curvature of the light response.

A is then calculated as:

$$A = \min(A_c, A_j, A_e) \qquad (5)$$

Eqns. 1 and 2 may take the general form:

$$A = \gamma \frac{(C_c - \Gamma^*)}{(C_c + \beta_A)} \quad (6)$$

where $\gamma = V_{cmax}$ (Rubisco-limited photosynthesis, A_c) or $J/4$ (Light-limited photosynthesis, A_j) and $\beta_A = K_c(1 + O_i / K_o)$ (Rubisco-limited photosynthesis, A_c) or $2\,\Gamma^*$ (Light-limited photosynthesis, A_j).

Stomatal conductance sub-model

The semi-empirical approach described in Jacobs et al. (1996) was used. The model can be expressed as:

$$g_{sc} = g_0 + m \frac{A}{(C_s - \Gamma)\left(1 + \frac{D_s}{D^*}\right)} \quad (7)$$

where g_{sc} (mol m^{-2} s^{-1}) is the stomatal conductance to CO_2, g_0 (mol m^{-2} s^{-1}) is the cuticular conductance, Γ is the CO_2 compensation point (µmol mol^{-1}), C_s (µmol mol^{-1}) is the CO_2 concentration at the leaf surface, D_s is the vapour pressure deficit at the leaf surface, m is equal to $1/(1-f_0)$ and D^* is $D_{max}/(m-1)$; f_0 and D_{max} being the parameters defined by Jacobs et al. (1996).

Eqns 6 and 7 have three unknowns (A, C_c and g_{sc}), provided that D_s and C_s are known or assumed equal to the bulk air' values. To obtain an analytical solution for A and g_{sc} we need an equal number of equations and unknowns. A simple conductance relation can be expressed to relate A and g_{sc}:

$$A = g_t\,(C_s - C_c^*) \quad (8)$$

where g_t (mol m^{-2} s^{-1}) = (g_{sc} x g_m) / (g_{sc} + g_m), g_m is the mesophyll conductance to CO_2 diffusion (mol m^{-2} s^{-1}) and C_c^* is the chloroplastic CO_2 concentration (µmol mol^{-1}). Note that the units of C_c in Eqns 8 and 6 are different:

C_c^* (µmol mol^{-1}) = C_c (Pa) / P

P being the conversion factor.

Water stress

The effect of water stress is incorporated by applying a soil-moisture dependent function to m (Eqn. 7, β_S), to g_m (Eqn. 8, β_M) and to the parameters J_{max} and V_{cmax} (Eqn. 6, β_B). The three water stress functions, β_S, β_M and β_B, were given the following form:

$$\beta_i = \begin{cases} 1 & \theta \geq \theta_c \\ \left[\frac{\theta - \theta_w}{\theta_c - \theta_w}\right]^{q_j} & \theta_w < \theta < \theta_c \\ 0 & \theta \leq \theta_w \end{cases} \quad (9)$$

where β_i is a soil moisture dependent function ranging from 1 (for plants not suffering from water stress) to 0 (for wilting plants). The subscript i,j = S, M and B are for stomatal, mesophyll and biochemical limitations, respectively. The extra degree of freedom in subscript j in the q_j exponent enables the imposition of combinations of multiple β pathways to a single experiment.

Derivation

Now that the set of working equations has been articulated, the next step is to derive an equation describing C_c that is independent of g_{sc} and A. The term g_{sc} is eliminated by inserting Eqn. 7 in Eqn. 8. Subsequently, the term A is eliminated by inserting Eqn. 6 into the resulting equation. After algebraic manipulation, an expression for C_c is derived:

$$\mathrm{A}C_c^3 + \mathrm{B}C_c^2 + \mathrm{C}C_c + \mathrm{D} = 0 \qquad (10)$$

where

$$\mathrm{A} = g_0\, g_m + \mathrm{X}\, \gamma\, g_m\, \mathrm{P}^{-1} - \mathrm{X}\, R_d\, g_m\, \mathrm{P}^{-1}$$

$$\mathrm{B} = \gamma\, g_0 + \mathrm{X}\, \gamma^2 - \mathrm{X}\, \gamma R_d + \gamma\, g_m - R_d\, g_0 - \mathrm{X}\, \gamma R_d + \mathrm{X}\, R_d^2 - g_m\, R_d - g_0\, g_m\, C_s - \mathrm{X}\, g_m\, \gamma\, C_s + \mathrm{X}\, g_m\, R_d\, C_s + 2\, g_0\, g_m\, \mathrm{P}^{-1}\, \beta + \mathrm{X}\, g_m\, \gamma\, \mathrm{P}^{-1}\, \beta - \mathrm{X}\, g_m\, \gamma\, \mathrm{P}^{-1}\, \Gamma^* - 2\, \mathrm{X}\, g_m\, R_d\, \mathrm{P}^{-1}\, \beta$$

$$\mathrm{C} = g_0\, \gamma\, \beta - g_0\, \gamma\, \Gamma^* - 2\, \mathrm{X}\, \gamma^2\, \Gamma^* - \mathrm{X}\, \gamma R_d\, \beta + \mathrm{X}\, \gamma R_d\, \Gamma^* + g_m\, \gamma\, \beta - g_m\, \gamma\, \Gamma^* - 2\, g_0\, R_d\, \beta - \mathrm{X}\, \gamma R_d\, \beta + \mathrm{X}\, \gamma R_d\, \Gamma^* + 2\, \mathrm{X}\, R_d^2\, \beta - 2\, g_m\, R_d\, \beta - 2\, g_0\, g_m\, C_s\, \beta - \mathrm{X}\, g_m\, \gamma\, C_s\, \beta + \mathrm{X}\, g_m\, \gamma\, C_s\, \Gamma^* + 2\, \mathrm{X}\, g_m\, R_d\, C_s\, \beta + g_0\, g_m\, \mathrm{P}^{-1} \beta^2 - \mathrm{X}\, g_m\, \gamma\, \mathrm{P}^{-1}\, \Gamma^* \beta - \mathrm{X}\, g_m\, R_d\, \mathrm{P}^{-1} \beta^2$$

$$\mathrm{D} = -\, g_0\, \gamma\, \Gamma^*\, \beta + \mathrm{X}\, \gamma^2\, \Gamma^{*2} + \mathrm{X}\, \gamma\, R_d\, \Gamma^*\, \beta - g_m\, \gamma\, \Gamma^*\, \beta - g_0\, R_d\, \beta^2 + \mathrm{X}\, R_d\, \gamma\, \Gamma^* \beta + \mathrm{X}\, R_d^2\, \beta^2 - R_d\, g_m\, \beta^2 - g_0\, g_m\, C_s\, \beta^2 + \mathrm{X}\, g_m\, \gamma\, C_s\, \beta\, \Gamma^* + \mathrm{X}\, R_d\, g_m\, C_s\, \beta^2$$

where $\mathrm{X} = m\,(C_s - \Gamma)^{-1}\,(1 + D_s/D_0)^{-1}$

Solution

The solution of the cubic equation is taken from Baldocchi (1994) who took it from Press et al. (1989). Eqn 10 must be manipulated into the form:

$$C_c^3 + \mathrm{b}C_c^2 + \mathrm{c}C_c + \mathrm{d} = 0 \qquad (11)$$

by doing:

$\mathrm{b}=\mathrm{B}/\mathrm{A}$

$\mathrm{c} = \mathrm{C}/\mathrm{A}$

$\mathrm{d} = \mathrm{D}/\mathrm{A}$

the roots for Eqn 11 are:

$$C_{c}\_1 = -2\sqrt{Q}\cos\left(\frac{\varepsilon}{3}\right) - \frac{p}{3}$$

$C_{c}\_2 = -2\sqrt{Q}cos\left(\frac{\varepsilon+2\pi}{3}\right) - \frac{p}{3}$

$C_{c}\_3 = -2\sqrt{Q}cos\left(\frac{\varepsilon+4\pi}{3}\right) - \frac{p}{3}$

where:

$$Q = \frac{p^2 - 3q}{9}$$

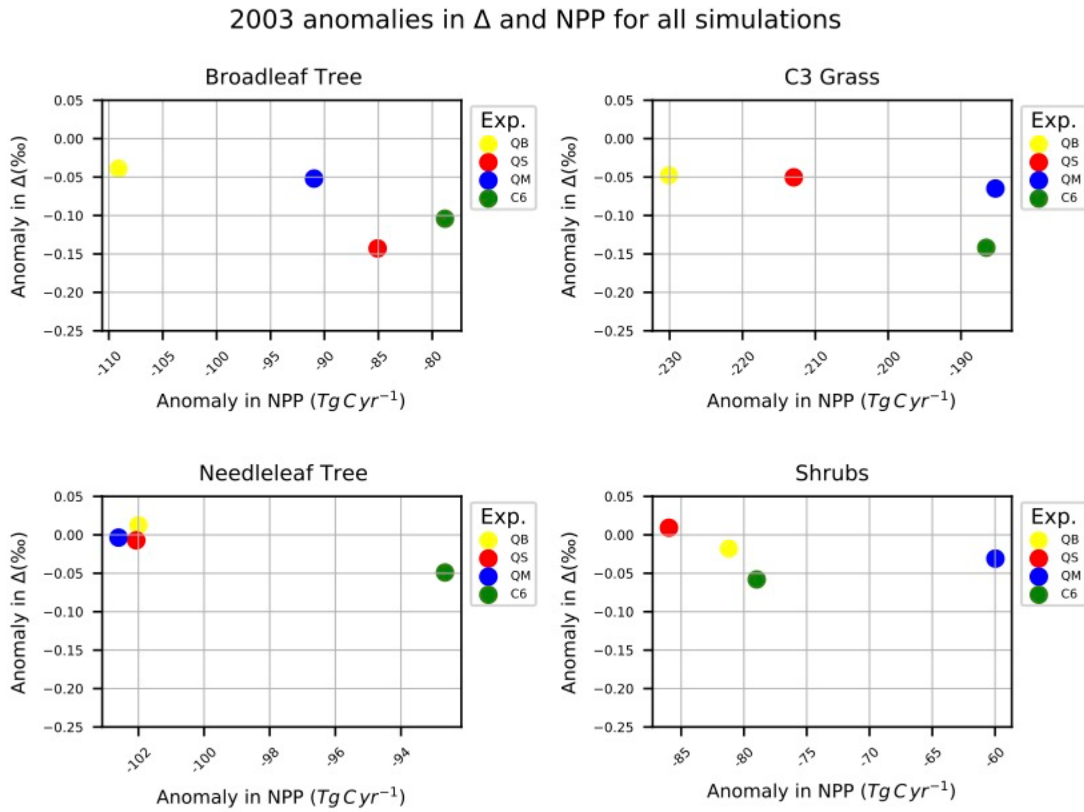
$$R = \frac{2p^3 - 9pq + 27r}{54}$$

$$\varepsilon = acos\left(\frac{R}{\sqrt{Q^3}}\right)$$

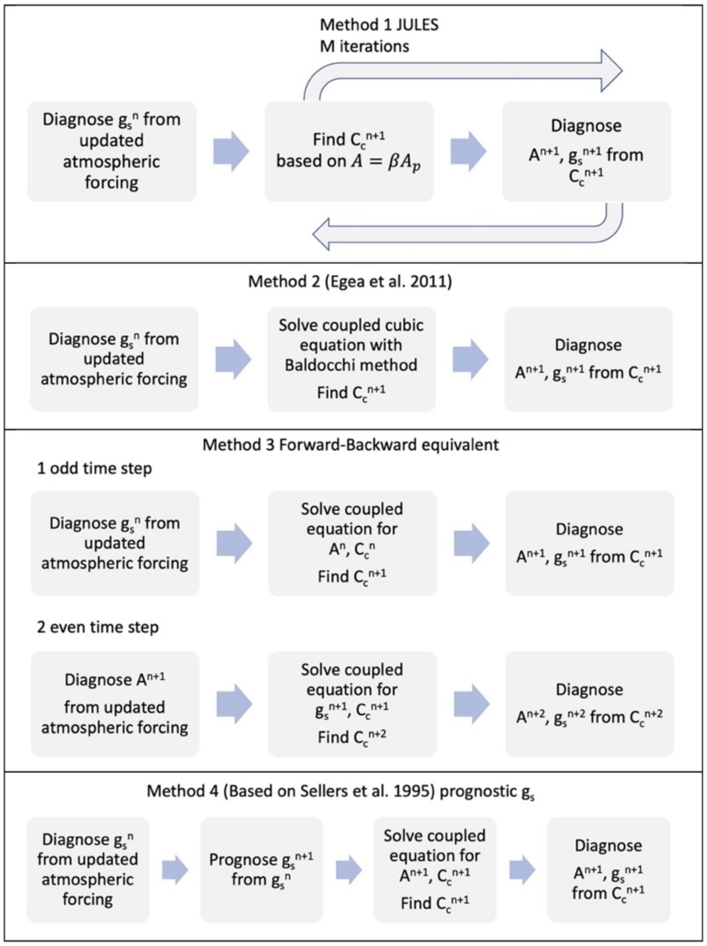
The right value for C_c corresponds to root number two (C_c_2). Equation 11 must be solved twice: the first time to compute the limitation of A by Rubisco activity ($\gamma = V_{cmax}$; $\beta = K_c(1 + O_i / K_o)$), the second time to compute the limitation of A by RuBP regeneration ($\gamma = J/4$; $\beta = 2\Gamma^*$). Once A_c and A_j are determined (Eqn. 6), A is calculated with Eqn. 5 and g_{sc} is then determined with Eqn. 7.

2 Supplementary Figures and Tables

2.1 Supplementary Figures



Supplementary Figure 1. The NPP (Tg C yr^{-1}) and Δ (‰) anomalies for the year 2003 in Europe. This figure is similar to the inset in Fig. 3 of Peters et al. (2018), albeit showing the anomaly in NPP instead of NEE, and including individual panels for each plant functional type.



Supplementary Figure 2. A summary of the numerical solution methods used in JULES (Method 1, top row) for the CTL experiment and the Egea (2011) methods (Method 2, 2nd row) used for experiments QB, QS, QM and C6. Two more methods are introduced as possible research and development avenues: methods 3 and 4, bottom rows.