

Appendix F. The Farquhar Photosynthesis & Ball-Berry model.

Overview

Photosynthesis is described using a system of 3 equations in 3 unknowns; net rate of leaf photosynthesis (A), stomatal conductance (g_s), and intercellular partial pressure of CO₂ (C_i), whereby they all influence each other. We used the following equations; Farquhar's non-linear equation (A vs C_i), Ball-Berry equation (g_s vs A) and the diffusion equation ($A = g_s (C_a - C_i)$). We solved all of these equations simultaneously by taking an iterative approach ([Leuning 1990](#), [Collatz et al. 1991](#), [Harley et al. 1992](#)). The detailed algorithm for modeling photosynthesis is described below.

Modelling Photosynthesis

Both CO₂ and O₂ compete for Rubisco binding site in the processes known as carboxylation and oxygenation, respectively ([Farquhar et al. 1980](#)). To account for the competitive inhibition between CO₂ and O₂, net rate of leaf photosynthesis (A) is mathematically expressed as

$$A = W_c - 0.5W_o - R_d = W_c \left(1 - \frac{0.5O}{\tau C_i}\right) - R_d, \quad (\text{F.1})$$

where W_c and W_o are the rates of carboxylation and oxygenation, respectively, and R_d is the mitochondrial respiration in the light, which is considered as $0.015 * V_{c,max}$ ([Farquhar et al. 1980](#)). The factor 0.5 reflects the fact that for each two oxygenations of Rubisco, one molecule of CO₂ is released in photorespiration. The specificity factor for Rubisco ([Jordan and Ogren 1984](#)) is designated τ , while C_i and O are the partial pressures of CO₂ and O₂ in the intercellular air space, respectively.

The rate at which Rubisco is carboxylated (i.e. W_c) depends upon (i) the amount, activity, and kinetic properties of Rubisco, and (ii) the rate of ribulose-1,5 bisphosphate (RuBP) regeneration via electron transport. Combining Eq. F.1 with the concept that carboxylation is regulated by the 'minimum' of these two limiting conditions yields the expression,

$$A = \min(W_c, W_j) - R_d = \left(1 - \frac{0.5O}{\tau C_i}\right) \min(W_c, W_j) - R_d \quad (\text{F.2})$$

In the text below, we describe the exact version of equations for calculating W_c and W_j , which were used in different studies.

Version 1

We use version 1 as the reference version – this version has been used by Wullschleger (1993) across a large variety of plant species. When the rate of carboxylation is limited solely by the amount, activation state, and kinetic properties of Rubisco, carboxylation can be described by,

$$W_c = V_{c,max} \frac{C_i}{C_i + K_c(1 + O/K_o)} \quad (\text{F.3})$$

where $V_{c,max}$ is the maximum rate of carboxylation, competitive with respect to both CO₂ and oxygen, and K_c and K_o are Michaelis constants for carboxylation and oxygenation, respectively. Likewise, when carboxylation is limited solely by the regeneration of RuBP via electron transport, the rate of carboxylation can be expressed by,

$$W_j = J \frac{C_i}{4(C_i + O/\tau)} \quad (\text{F.4})$$

where J is the potential rate of electron transport, and the factor 4 indicates that the transport of four electrons will generate sufficient ATP and NADPH for the regeneration of RuBP in the Calvin cycle ([Farquhar and von Caemmerer 1982](#)). The potential rate of electron transport is dependent upon irradiance, I , according to the empirical expression of Smith ([1937](#)),

$$J = \frac{\alpha I}{\left(1 + \frac{\alpha^2 I^2}{J_{max}^2}\right)^{1/2}}$$

where α , the efficiency of light energy conversion is considered as 0.25 (unitless) ([Niinemets and Tenhunen 1997](#)) and J_{max} is the light-saturated rate of electron transport.

Version 2

Some studies used Version 2 (see Table A1). Here, when A is Rubisco limited the velocity of carboxylation can be expressed as

$$W_c = V_{c,max} \frac{C_i - \frac{0.5O}{\tau}}{C_i + K_c \left(1 + \frac{O}{K_o}\right)}, \text{ provided } C_i > 0.5O/\tau \quad (\text{F.5})$$

while the electron-transport limited rate of photosynthesis is given by

$$W_j = J \frac{C_i - \frac{0.5O}{\tau}}{4\left(C_i + 2\frac{0.5O}{\tau}\right)}, \text{ provided } C_i > 0.5O/\tau \quad (\text{F.6})$$

Ball-Berry Model

The stomatal conductance (g , m/s) was evaluated by the Ball-Berry empirical stomatal conductance model ([Ball et al. 1987](#)):

$$g = g_0 + m \frac{A \cdot RH}{C_a} \quad (\text{F.7})$$

where RH is the relative humidity (unitless) at the leaf surface, C_a is the CO₂ concentration at the leaf surface, and g_0 and m are the minimum stomatal conductance (0.0005 m/s) and the slope, respectively.

The estimation of A could be sensitive to the choice of maximum stomatal conductance slope, which we set the same for all species, despite the evidence that this parameter varies both within and across species ([Harley and Baldocchi 1995](#), [Wilson et al. 2001](#)). A recent synthesis provides the first analysis of the global variation in stomatal slope based on an alternative algorithm that considers representation of optimal stomatal behavior ([Lin et al. 2015](#)). However, following CLM4.5, which uses the Ball-Berry empirical stomatal conductance model ([Ball et al. 1987](#)), we fixed the value of stomatal slope (m) as 9 for all PFTs in our study.

Calculation of photosynthetic rate

Using Eqs. F.3 and F.4, photosynthetic rate (A) was determined by solving Eqs. F.2 and F.7 simultaneously by taking an iterative approach ([Leuning 1990](#), [Collatz et al. 1991](#), [Harley et al. 1992](#)). The following steps were followed:

- 1) Given the initial values of C_i (where initial value of C_i was assumed 0.7 x ambient CO₂ concentration), the temperature dependence functions of $V_{c,max}$ and J_{max} (see Appendix E), and the temperature dependence of Rubisco kinetics (O , τ , K_c and K_o , see Appendix D), A was calculated from equation F.2.

- 2) CO₂ concentration at the leaf surface (C_a) was determined by calculating the difference between C_i and the partial pressure due to A , wind speed and the dimension of the leaf.
- 3) Given A and C_a , and using equation F.7, stomatal conductance (g) was determined.
- 4) Next C_i was determined by calculating the difference between C_a and partial pressure due to A , boundary conditions of the stomata.
- 5) Using the leaf energy balance, leaf temperature was calculated. Then again steps 1-5 were executed.

The above four steps were repeated in a systematic way until g was equilibrated. The final value of A was then recorded.

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