

An analytical solution for coupled leaf photosynthesis and stomatal conductance models

DENNIS BALDOCCHI

Atmospheric Turbulence and Diffusion Division, NOAA, P.O. Box 2456, Oak Ridge, TN 37831, USA

Received August 16, 1993

Summary

Iterative solutions of coupled leaf photosynthesis and stomatal conductance equations sometimes yield bifurcated or chaotic solutions. An analytical solution for coupled leaf photosynthesis–stomatal conductance equations is preferred because an analytical model has specific and known roots, and partial derivatives can be taken to perform sensitivity analyses. I present an analytical solution for coupled leaf photosynthesis and stomatal conductance equations that are based on established biochemical and physiological theory.

Keywords: analytical model, chaos iterative model.

Introduction

A plethora of experimental evidence shows that leaf photosynthesis and stomatal conductance are linked (Wong et al. 1979, Farquhar and Sharkey 1982). In recent years, theoreticians have exploited this linkage to derive mathematical models of net photosynthesis (A) and stomatal conductance (g_s). Cowan and coworkers (Cowan and Troughton 1972, Cowan and Farquhar 1977, Cowan 1982) used optimization theory to describe the linkage between A and g_s . They argue that one function of optimal stomatal action is to minimize water loss for a given rate of carbon gain; mathematically, infinitesimal changes in g_s cause the partial derivative of transpiration (E) with respect to assimilation ($\partial E/\partial A$) to be constant. Experimental validation of this theory yields mixed results. Some workers show that $\partial E/\partial A$ is constant under controlled laboratory (Farquhar et al. 1980, Hall and Schulze 1980, Meinzer 1982) and field conditions (Field et al. 1982), whereas others report that $\partial E/\partial A$ is variable in the field (Fites and Teskey 1988).

The optimization theory of Cowan and coworkers is appealing because it simulates unique features of diurnal leaf gas exchange, such as midday stomatal closure. On the other hand, this theory may be perceived as impractical because it is unable to prescribe a unique optimization coefficient (Cowan and Farquhar 1977, Farquhar and Sharkey 1982).

The physiological ecology community needs a practical and valid leaf photosynthesis and stomatal conductance model for scaling CO_2 and water vapor fluxes from leaf to canopy scales. Several candidate models exist that exploit empirical links between stomatal action and environmental and biological signals. For example, several teams have modeled stomatal conductance as a slave to leaf photosynthesis

(Norman 1982, Farquhar and Wong 1984, Leuning 1990, Collatz et al. 1991, Harley et al. 1992). The foundation of this approach is based on the work of Wong et al. (1979), who hypothesized that stomata sense the intercellular CO_2 concentration (C_i) (a variable that depends on leaf photosynthesis) because stomata open or close to maintain either C_i or the ratio between C_i and the ambient CO_2 concentration (C_a) at a constant level. A derivative of this approach was proposed by Ball (1988) and implemented by Collatz et al. (1991) and Leuning (1990). They modeled stomatal conductance as a function of leaf photosynthesis, leaf surface relative humidity (rh), and the surface CO_2 concentration (C_s). Ball's stomatal conductance model is appealing because its variables can be determined from mechanistic photosynthesis (Farquhar et al. 1980, Farquhar and von Caemmerer 1982) and leaf energy balance models. Another strength of coupling stomatal conductance to photosynthesis is an ability to vary stomatal conductance as a function of nutrient and CO_2 availability, factors that determine photosynthetic capacity (Wong et al. 1979, 1985, Field and Mooney 1986, Harley et al. 1992).

Given a system of equations describing photosynthesis and stomatal conductance, one has the task of solving a set of non-linear and coupled equations. Past modeling exercises have solved coupled equations for A and g_s by iteration (Leuning 1990, Collatz et al. 1991, Harley et al. 1992). This approach is not always ideal because iterative solutions of non-linear biological systems can behave chaotically or oscillate if model parameters exceed certain values (May 1976). I found that iterative solutions for A became unstable when the leaf boundary layer resistance and the CO_2 compensation point exceeded critical values. For example, iterative solutions for A bifurcated when the leaf boundary layer resistance equalled 500 s m^{-1} (Figure 1),

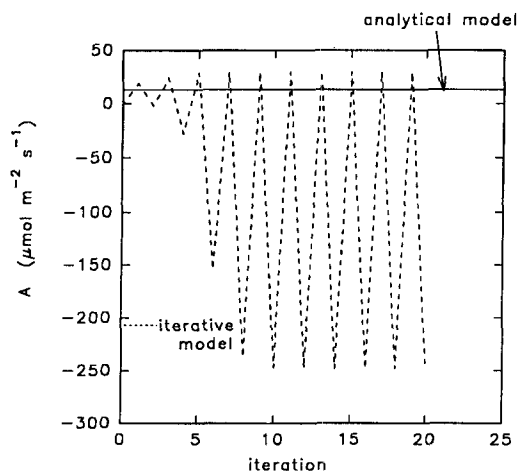


Figure 1. Comparison between the analytical and iterative solution for leaf photosynthesis. Under environmental conditions where $[\text{CO}_2]$ equals 300 ppm, air temperature equals 30°C , photosynthetic photon flux density equals $1000 \mu\text{mol m}^{-2} \text{ s}^{-1}$, the CO_2 compensation point equals 35 ppm and leaf boundary layer resistance equals 500 s m^{-1} , the iterative model bifurcates, whereas the analytical model yields a distinct root.

and under more extreme situations ($[\text{CO}_2] < 150$ ppm), numerical calculations of photosynthesis yielded chaotic solutions.

An analytical solution for the coupled leaf photosynthesis–stomatal conductance model is preferred because it has specific and known roots, its partial derivatives can be taken to perform a sensitivity analysis and, under some circumstances, an analytical solution arrives at its solution quicker than does an iterative method. The objective of this report is to describe the derivation of an analytical solution for coupled equations describing leaf photosynthesis (Farquhar et al. 1980, Farquhar and von Caemmerer 1982, Harley and Tenhunen 1991) and stomatal conductance (Ball 1988). A discussion of this analytical solution is also presented.

Theory

Leaf photosynthesis is a function of the carboxylation (V_c), oxygenation (V_o , photorespiration) and dark respiration (R_d) rates of CO_2 exchange between the leaf and the atmosphere.

$$A = V_c - 0.5V_o - R_d \quad (1)$$

The term $V_c - 0.5V_o$ is expressed by Farquhar et al. (1980) as

$$V_c - 0.5V_o = \min(W_j, W_c) \left(1 - \frac{\Gamma}{C_i} \right), \quad (2)$$

where W_c is the rate of carboxylation when ribulose bisphosphate (RuBP) carboxylase/oxygenase is saturated, W_j is the carboxylation rate when RuBP regeneration is limited by electron transport, $\min(W_j, W_c)$ is the minimum value between these two rate variables and Γ is the CO_2 compensation point in the absence of dark respiration. Both, W_j and W_c take the algebraic form (see Farquhar and von Caemmerer 1982, Harley and Tenhunen 1991)

$$\frac{aC_i - ad}{eC_i + b}, \quad (3)$$

where the variables a , b , c and d are defined later.

Introduction of Equation 3 yields a new unknown, C_i , the internal CO_2 concentration. To obtain an analytical solution for leaf photosynthesis, we need an equal number of equations and unknowns. A simple conductance relation can be employed to express C_i :

$$C_i = C_s - \frac{A}{g_s}. \quad (4)$$

Unfortunately, this equation produces two more unknowns, g_s (stomatal conductance) and C_s , for which additional expressions are needed. The CO_2 concentration

at the leaf's surface (C_s) can be expressed in terms of the atmosphere's CO_2 concentration (C_a) and the conductance across the laminar boundary layer of a leaf (g_b):

$$C_s = C_a - \frac{A}{g_b}. \quad (5)$$

Here, C_a and g_b are external inputs.

Finally, to close the system of equations and unknowns, an equation is needed to describe stomatal conductance, g_s . I chose the equation of Ball (1988) to represent g_s :

$$g_s = \frac{mA\rho h}{C_s} + b'. \quad (6)$$

The coefficient m is a dimensionless slope, ρh is relative humidity and b' is the zero intercept when A is equal to or less than zero. This function has been validated for many species (Leuning 1990, Collatz et al. 1991, Harley et al. 1992). An attraction of Equation 6 is its requirement for fewer tunable coefficients than other stomatal conductance models, e.g., Jarvis (1976). Weaknesses associated with Ball's stomatal model include its inability to force stomatal closure in response to water deficits. Aphalo and Jarvis (1991) also argue that stomata do not respond to relative humidity, but instead respond to the water vapor saturation deficit.

Derivation

Now that the set of working equations has been articulated, our goal is to derive an equation describing A that is independent of C_s , C_i and g_s . The term C_s is eliminated by inserting Equation 5 into Equations 4 and 6. Subsequently, the term g_s is eliminated by inserting Equation 6 into Equation 4; when applying Equation 6 to calculate photosynthesis, the reader must remember that it was derived for water vapor, so it must be divided by the ratio of molecular diffusivities of CO_2 and water vapor (1.6). After algebraic manipulation, an expression for C_i is derived:

$$C_i = \frac{(C_a g_b m \rho h A + C_a^2 b' g_b - C_a b' A) + \left(-A^2 m \rho h - A b' C_a + \frac{A^2 b'}{g_b} \right) + (-g_b A C_a + A^2)}{g_b m \rho h A + b' g_b C_a - b' A}. \quad (7)$$

Further algebraic manipulation yields a cubic equation dependent on A .

$$0 = e\alpha A^3 + A^2(e\beta + b\theta - a\alpha + e\alpha R_d) + A(e\gamma + \frac{b\gamma}{C_a} - a\beta + ad\theta + eR_d\beta + R_d b\theta) - a\gamma + \frac{ad\gamma}{C_a} + eR_d\gamma + \frac{R_d b\gamma}{C_a}. \quad (8)$$

The variables a , b , d , and e are coefficients from Equation 2. If W_c is minimal, these coefficients correspond to

$$V_c - 0.5V_o = \frac{aC_i - ad}{eC_i + b} = \frac{V_{\text{cmax}}(C_i - \Gamma)}{C_i + K_c \left(1 + \frac{[O_2]}{K_o}\right)}, \quad (9)$$

where V_{cmax} is the maximum carboxylation rate when RuBP carboxylase/oxygenase is saturated, K_o and K_c are the Michaelis-Menten coefficients for O_2 and CO_2 and Γ is the CO_2 compensation point in the absence of dark respiration. If W_j is minimal, the a , b , d and e coefficients correspond to

$$V_c - 0.5V_o = \frac{aC_i - ad}{eC_i + b} = \frac{J(C_i - \Gamma)}{4C_i + 8\Gamma}, \quad (10)$$

where J is the potential rate of electron transport. Other terms in Equation 8 are defined in the following equations:

$$\alpha = 1 + \frac{b'}{g_b} - mrh, \quad (11)$$

$$\beta = C_a(g_bmrh - 2b' - g_b), \quad (12)$$

$$\gamma = C_a^2 b' g_b, \quad (13)$$

and

$$\theta = g_bmrh - b'. \quad (14)$$

Solution

The solution of the cubic equation is taken from Press et al. (1989). Solutions published in other mathematical handbooks were intractable and did not yield roots that corresponded with the iterative solution. In brief, if Equation 8 is manipulated into the form

$$x^3 + px^2 + qx + r = 0, \quad (15)$$

three roots for the cubic equation are

$$x_1 = -2\sqrt{Q} \cos\left(\frac{\theta}{3}\right) - \frac{p}{3},$$

$$x_2 = -2\sqrt{Q} \cos\left(\frac{\theta + 2\pi}{3}\right) - \frac{p}{3},$$

and

$$x_3 = -2\sqrt{Q} \cos\left(\frac{\theta + 4\pi}{3}\right) - \frac{p}{3}. \quad (16)$$

Terms in Equation 16 are defined as

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

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

and

$$\theta = \arccos\left(\frac{R}{\sqrt{Q^3}}\right). \quad (17)$$

The photosynthetic flux density of a leaf (A) corresponds to root number three (x_3). Sensitivity tests reveal that this root is correct for a wide range of environmental conditions that are commonly encountered in the field. The solution was tested for photosynthetically active radiation flux densities (PAR) between 0 and 2000 $\mu\text{mol m}^{-2} \text{s}^{-1}$, $[\text{CO}_2]$ between 50 and 650 ppm, leaf temperatures (T_l) between 5 and 35 °C and leaf boundary layer resistances (r_b) between 1 and 2000 s m^{-1} .

Discussion

Many studies have verified that the applied system of gas exchange equations (Equations 1, 4, 5 and 6) predicts leaf photosynthetic rates and stomatal conductances (e.g., Leuning 1990, Collatz et al. 1991, Harley et al. 1992). But it is not known whether the iterative and analytical models yield similar results when the iterative model is tractable. Figure 2 shows that the two model schemes yielded identical results for a wide range of environmental conditions. On the other hand, divergence between analytical and iterative solutions of A can occur on a sunny day, for instance, when the boundary layer resistance (the inverse of conductance) is low (less than 1 s m^{-1}) or large (greater than 500 s m^{-1}) (Figure 3).

The sensitivity of the analytical solution to environmental forcing was examined. Figure 4 shows that model calculations of A increase with PAR and CO_2 concentration, as do data published in the literature (Farquhar and von Caemmerer 1982, Harley et al. 1992). When CO_2 concentrations were below 650 ppm, A increased with PAR until an inflection occurred. Thereafter, A was insensitive to changes in PAR. This inflection reflects the fact that A was limited by W_j when PAR was below a threshold, and A was limited by W_c and the availability of CO_2 when PAR exceeded a threshold. Quantum yields (the initial slope of Figure 4) and photosynthetic

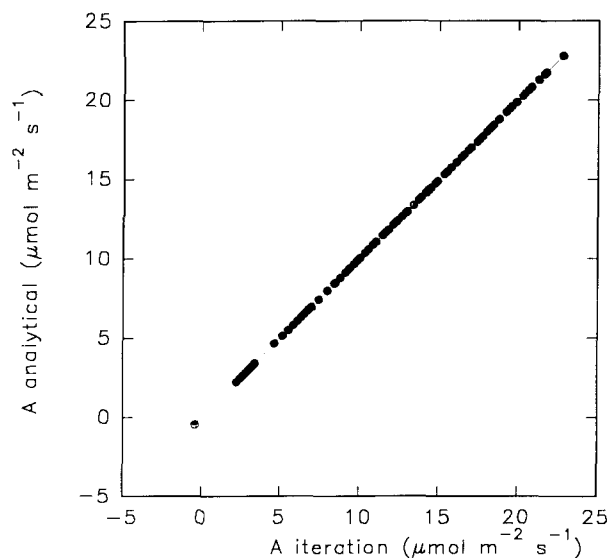


Figure 2. A comparison between leaf photosynthetic flux densities computed with the analytical model (A_{cubic}) and the numerical iterative model (A_{iterated}). C_a varied from 150 to 1050 ppm and the photosynthetic photon flux density varied from 0 to 2000 $\mu\text{mol m}^{-2} \text{s}^{-1}$. The zero intercept equals 0.0006, the slope equals 0.9999 and the correlation coefficient equals 1.00. The biochemical rate coefficients were determined for a *Quercus alba* leaf by Peter Harley (unpublished data).

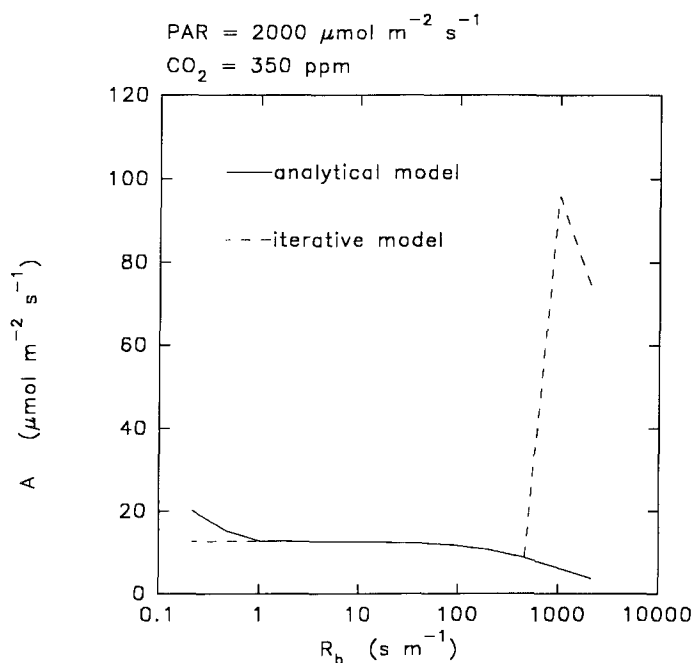


Figure 3. Calculation of leaf photosynthesis, using an analytical and a numerical method, while varying the leaf boundary layer resistance. The photosynthetic photon flux density was 2000 $\mu\text{mol m}^{-2} \text{s}^{-1}$, air temperature was 20 °C and the CO_2 concentration was 350 ppm.

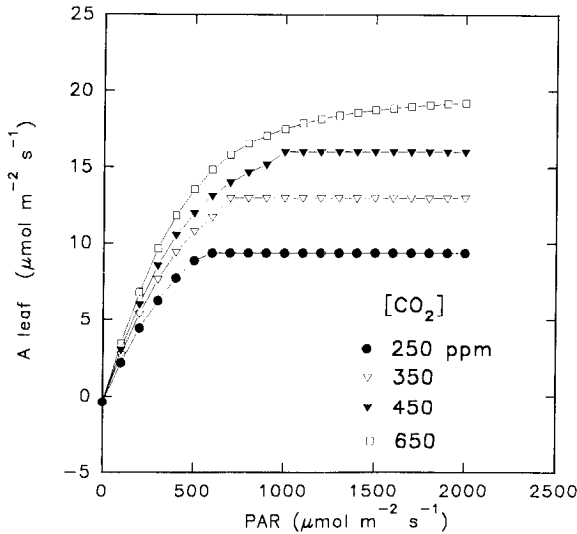


Figure 4. Calculations of the response of leaf photosynthesis to variations in CO_2 concentration and photosynthetic photon flux density (PAR).

capacity (maximum A) responded positively to increasing CO_2 concentrations, but the rate of change of these increases diminished with increasing CO_2 concentration.

Figure 5 shows the dependence of g_s on incoming PAR and CO_2 . Hereto, g_s has a curvilinear dependence on PAR. Although g_s is linearly dependent on A (Equation 6) (which responds positively to increasing CO_2), the net effect of changing CO_2 on g_s is a decrease of maximum conductance values with increasing CO_2 concentration.

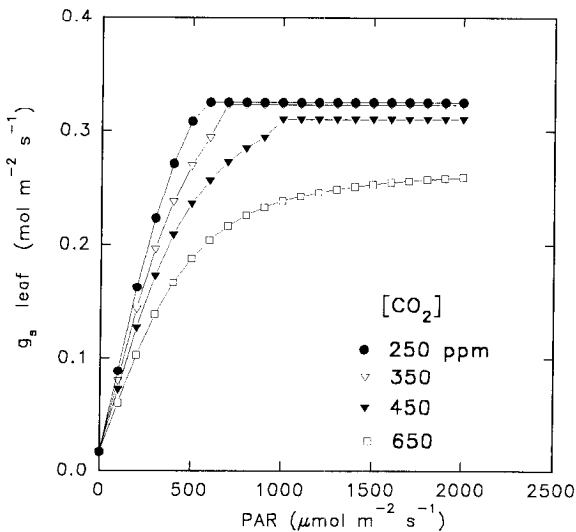


Figure 5. Calculations of the response of leaf stomatal conductances to variations in CO_2 concentration and photosynthetic photon flux density (PAR).

Mechanistic models can be used as tools to examine theoretical questions concerning the development of simpler parameterizations that are often needed for routine applications. Norman (1982) hypothesized that one can simplify the modeling of A by assuming that stomata open or close to maintain a constant C_i/C_a ratio. Figure 6 shows that C_i/C_a remains conservative (between 0.6 and 0.7) for a wide range of stomatal conductances. Only as stomata close does the ratio approach and exceed one, when photosynthesis diminishes and respiration rates overtake gross photosynthesis rates. In conclusion, Norman's assumption (Norman 1982) is valid over a wide range of environmental conditions, but is susceptible to failure as stomata close under low PAR.

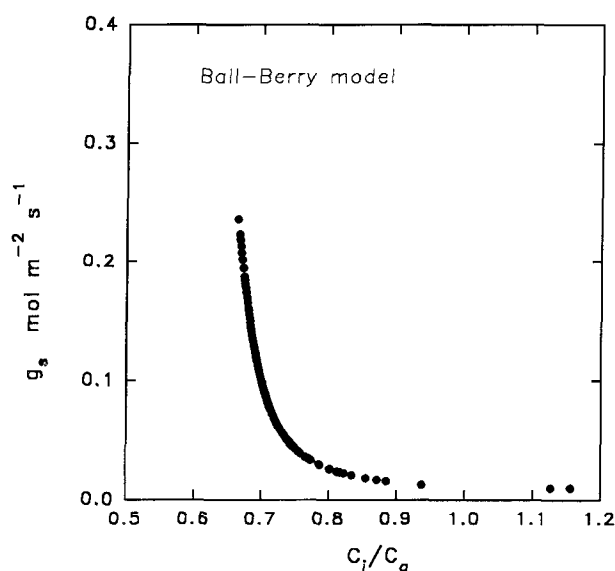


Figure 6. Correlation between calculations of leaf stomatal conductance and the ratio C_i/C_a .

Conclusion

A coupled analytical model for computing leaf photosynthesis and stomatal conductance was derived. Leaf photosynthesis is computed by solving a cubic equation. This scheme has an advantage over previous iterative routines, which yield bifurcated or chaotic solutions under specific conditions. One appeal of using a coupled photosynthesis–stomatal conductance model is its ability to scale stomatal conductance as a function of photosynthetic resources, irrespective of whether they are due to differences in soil or leaf nitrogen content or ambient CO_2 . An analytical leaf photosynthesis model, with defined roots, is also of particular use to the ecological modeling community. An integrated canopy photosynthesis model cannot afford to

use algorithms that yield intractable results under environmental conditions commonly encountered at various levels in the canopy.

Acknowledgment

This work was performed while the author was a 1992 RAISA Visiting Research Fellow at Università Della Tuscia, Viterbo, Italia. I am grateful to Dr. Riccardo Valentini and his colleagues at DISAFRI for their hospitality and scientific input. I thank my wife, Nicole, for allowing me to partake this Italian sojourn, and I thank Drs. Paul Hansen, Chris Vogel and Peter Harley for their constructive reviews and comments on this work.

References

- Aphalo, P.J. and P.G. Jarvis. 1991. Do stomata respond to relative humidity? *Plant Cell Environ.* 14:127–132.
- Ball, J.T. 1988. An analysis of stomatal conductance. Ph.D. Thesis, Stanford University, CA, 89 p.
- Collatz, G.J., J.T. Ball, C. Grivet and J.A. Berry. 1991. Regulation of stomatal conductance and transpiration: a physiological model of canopy processes. *Agric. For. Meteorol.* 54:107–136.
- Cowan, I.R. 1982. Regulation of water use in relation to carbon gain in higher plants. *In Encyclopedia of Plant Physiology*, Vol. 12B. Eds. O.L. Lange, P.S. Nobel, C.B. Osmond and H. Ziegler. Springer-Verlag, Berlin, pp 589–614.
- Cowan, I.R. and J.H. Troughton. 1972. The relative role of stomata in transpiration and assimilation. *Planta* 106:185–189.
- Cowan, I.R. and G.D. Farquhar. 1977. Stomatal function in relation to leaf metabolism and environment. *In Integration of Activity in the Higher Plant*. Ed. D.H. Jennings. Cambridge University Press, pp 471–505.
- Farquhar, G.D. and S. von Caemmerer. 1982. Modeling photosynthetic response to environmental conditions. *In Encyclopedia of Plant Physiology*, Vol. 12B. Eds. O.L. Lange, P.S. Nobel, C.B. Osmond and H. Ziegler. Springer-Verlag, Berlin, pp 549–587.
- Farquhar, G.D. and S.C. Wong. 1984. An empirical model of stomatal conductance. *Aust. J. Plant Physiol.* 11:191–210.
- Farquhar, G.D. and T.D. Sharkey. 1982. Stomatal conductance and photosynthesis. *Annu. Rev. Plant Physiol.* 33:317–45.
- Farquhar, G.D., S. von Caemmerer and J.A. Berry. 1980. A biochemical model of photosynthetic CO₂ assimilation in leaves of C₃ species. *Planta* 149:78–90.
- Farquhar, G.D., E.-D. Schulze and M. Koppers. 1980. Responses to humidity by stomata of *Nicotiana glauca* L. and *Corylus avellana* L. are consistent with the optimization of carbon dioxide uptake with respect to water loss. *Aust. J. Plant Physiol.* 7:315–327.
- Field, C. and H.A. Mooney. 1986. The photosynthesis–nitrogen relationship in wild plants. *In On the Economy of Plant Form and Function*. Ed. T.J. Givnish. Cambridge Press, pp 25–55.
- Field, C.B., J.A. Berry and H.A. Mooney. 1982. A portable system for measuring carbon dioxide and water vapor exchange of leaves. *Plant Cell Environ.* 5:179–186.
- Fites, J.A. and R.O. Teskey. 1988. CO₂ and water vapor exchange of *Pinus taeda* in relation to stomatal behavior: test of an optimization theory. *Can. J. For. Res.* 18:150–157.
- Hall, A.E. and E.-D. Schulze. 1980. Stomatal response to environment and a possible interrelation between stomatal effects on transpiration and CO₂ assimilation. *Plant Cell Environ.* 3:467–474.
- Harley, P.C. and J.D. Tenhunen. 1991. Modeling the photosynthetic response of C₃ leaves to environmental factors. *In Modeling Crop Photosynthesis from Biochemistry to Canopy*. American Society of Agronomy, Madison, WI, pp 17–39.
- Harley, P.C., R.B. Thomas, J.F. Reynolds and B.R. Strain. 1992. Modelling photosynthesis of cotton grown in elevated CO₂. *Plant Cell Environ.* 15:271–282.
- Jarvis, P.G. 1976. The interpretation of the variations in leaf water potential and stomatal conductance found in canopies in the field. *Phil. Trans. Roy. Soc. London B*273:593–610.
- Leuning, R. 1990. Modeling stomatal behavior and photosynthesis of *Eucalyptus grandis*. *Aust. J. Plant Physiol.* 17:159–175.

- May, R.M. 1976. Simple mathematical models with very complicated dynamics. *Nature* 261:459–467.
- Meinzer, F.C. 1982. The effect of vapor pressure on stomatal control of gas exchange in Douglas-fir (*Pseudotsuga menziesii*) saplings. *Oecologia* 54:236–242.
- Norman, J.M. 1982. Simulation of microclimates. *In* Biometeorology in Integrated Pest Management. Eds. J.L. Hatfield and I. Thompson. Academic Press, New York, pp 65–99.
- Press, W.H., B.P. Flannery, S.A. Teukolsky and W.T. Vetterling. 1989. Numerical recipes: the art of scientific computing. Cambridge University Press, Cambridge, U.K., 992 p.
- Wong, S.C., I.R. Cowan and G.D. Farquhar. 1979. Stomatal conductance correlates with photosynthetic capacity. *Nature* 282:424–426.
- Wong, S.C., I.R. Cowan and G.D. Farquhar. 1985. Leaf conductance in relation to rate of CO₂ assimilation. *Plant Physiol.* 78:821–825.

