# An analytical solution for coupled leaf photosynthesis and stomata conductance models

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# An analytical solution for coupled leaf photosynthesis and stomatal conductance models

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**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),
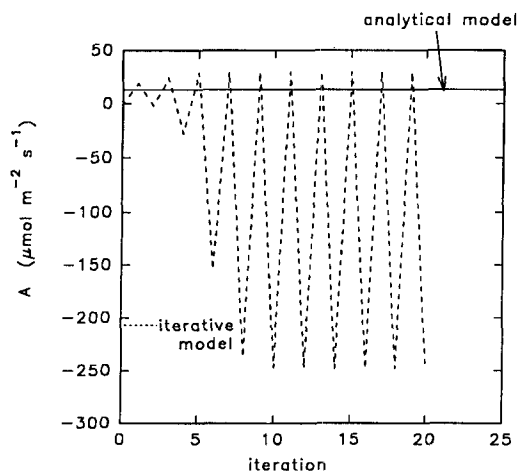


Figure 1. Comparison between the analytical and iterative solution for leaf photosynthesis. Under environmental conditions where [$CO_2$] equals 300 ppm, air temperature equals 30 °C, photosynthetic photon flux density equals 1000 μmol m$^{-2}$ s$^{-1}$, the $CO_2$ compensation point equals 35 ppm and 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 ($[CO_2] < 150$ ppm), numerical calculations of photosynthesis yieldcd 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.

$$A = V_c - 0.5V_o - R_d \tag{1}$$

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

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

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 $\Gamma$ 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)

$$\frac{aC_i - ad}{eC_i + b}, \tag{3}$$

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 $C_i$:

$$C_i = C_s - \frac{A}{g_s}. \tag{4}$$

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 ($g_b$):

$$C_s = C_a - \frac{A}{g_b} . \tag{5}$$

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 $g_s$:

$$g_s = \frac{mA\text{rh}}{C_s} + b' . \tag{6}$$

The coefficient $m$ is a dimensionless slope, rh 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 diffusitivities of $CO_2$ and water vapor (1.6). After algebraic manipulation, an expression for $C_i$ is derived:

$$C_i = \frac{(C_a g_b m\text{rh}A + C_a^2 b' g_b - C_a b'A) + \left(-A^2 m\text{rh} - Ab'C_a + \frac{A^2 b'}{g_b}\right) + (-g_b AC_a + A^2)}{g_b m\text{rh}A + b' g_b C_a - b'A} . \tag{7}$$

Further algebraic manipulation yields a cubic equation dependent on $A$.

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

$$\left. + ad\theta + eR_d\beta + R_d b\theta\right) \quad - a\gamma + \frac{ad\gamma}{C_a} + eR_d\gamma + \frac{R_d b\gamma}{C_a} . \tag{8}$$

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

$$V_c - 0.5V_0 = \frac{aC_i - ad}{eC_i + b} = \frac{V_{cmax}(C_i - \Gamma)}{C_i + K_c\left(1 + \dfrac{[O_2]}{K_o}\right)} ,$$ (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 $\Gamma$ 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

$$V_c - 0.5V_0 = \frac{aC_i - ad}{eC_i + b} = \frac{J(C_i - \Gamma)}{4C_i + 8\Gamma} ,$$ (10)

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

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

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

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

and

$$\theta = g_b mrh - b'.$$ (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

$$x^3 + px^2 + qx + r = 0,$$ (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

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

Terms in Equation 16 are defined as

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

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

and

$$\theta = a\cos\left(\frac{R}{\sqrt{Q^3}}\right). \tag{17}$$

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 $\mu$mol $m^{-2}$ $s^{-1}$, [$CO_2$] 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
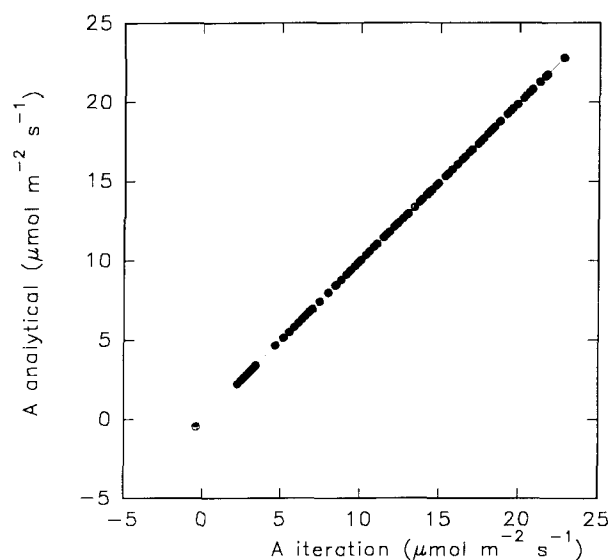
Figure 2. A comparison between leaf photosynthetic flux densities computed with the analytical model ($A_{cubic}$) and the numerical iterative model ($A_{iterated}$). $C_a$ varied from 150 to 1050 ppm and the photosynthetic photon flux density varied from 0 to 2000 $\mu$mol m$^{-2}$ s$^{-1}$. The zero 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).
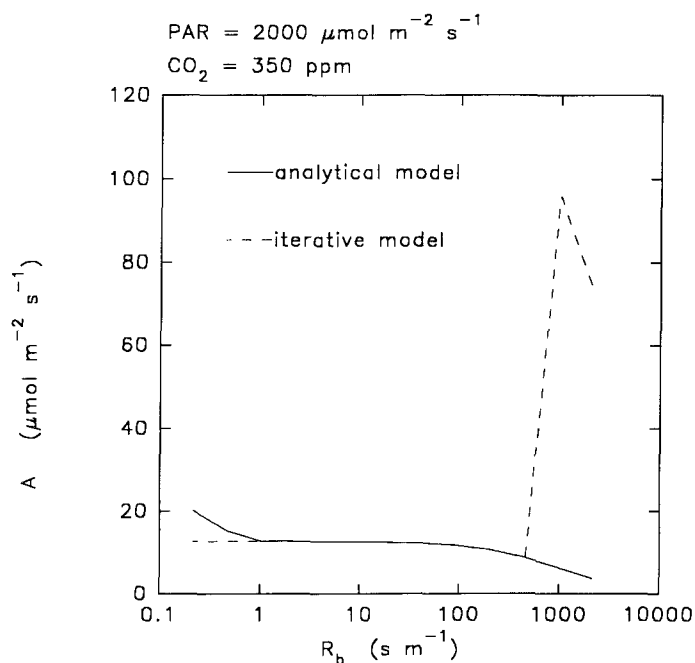


Figure 3. Calculation of leaf photosynthesis, using an analytical and a numerical method, while varying the leaf boundary layer resistance. The photosynthetic photon flux density was 2000 $\mu$mol m$^{-2}$ s$^{-1}$, air temperature was 20 °C and the $CO_2$ concentration was 350 ppm.
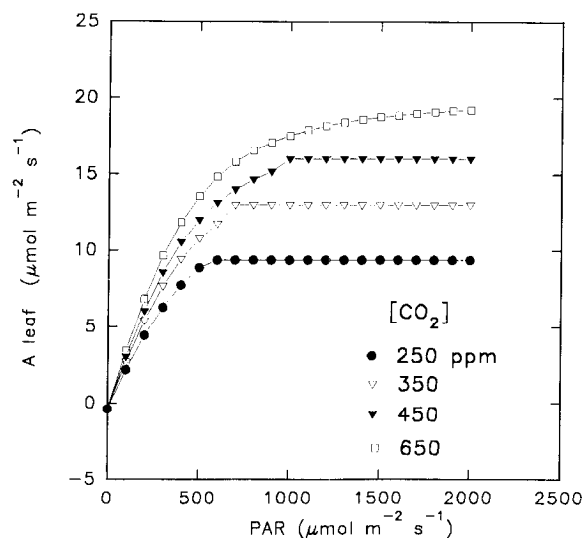
Figure 4. Calculations of the response of leaf photosynthesis to variations in $CO_2$ concentration and photosynthetic photon flux density (PAR).

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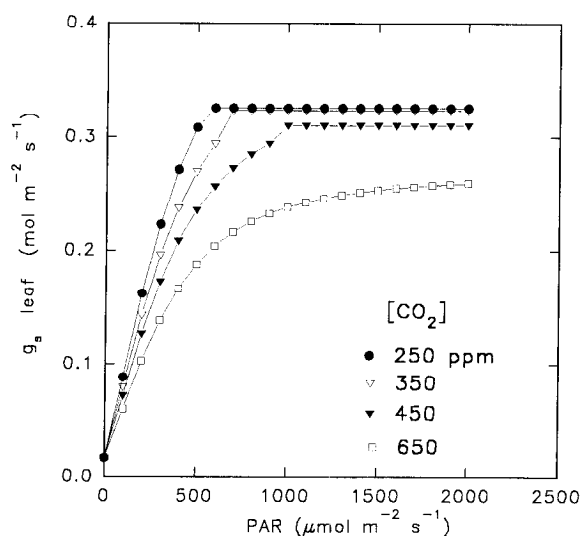
Figure 5. Calculations of the response of leaf stomatal conductances to variations in $CO_2$ concentration and photosynthetic photon flux density (PAR).

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.
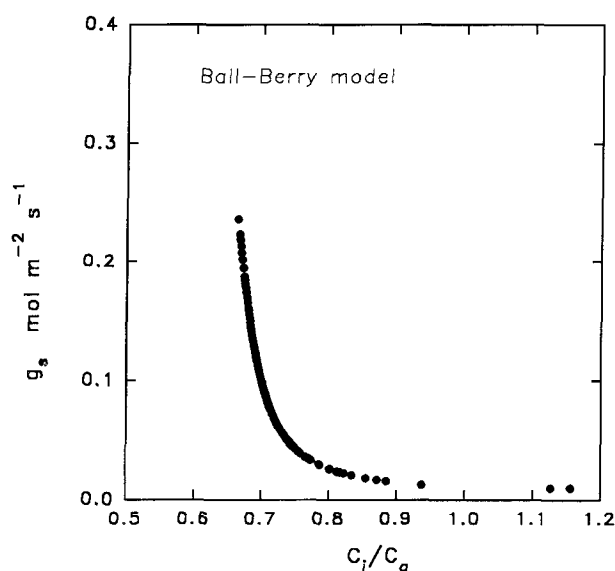


Figure 6. Correlation between calculations of leaf stomatal conductance and the ratio $C_i/C_a$.

## 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.

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