

A Comprehensive Model for CO₂ Assimilation in Leaves

R. H. Rand, J. R. Cooke
 ASSOC.
 MEMBER
 ASAE

ABSTRACT

A model of CO₂ assimilation in leaves is presented which includes consideration of the size and distribution of cells and biochemical kinetics. The model, which includes the effects of distributed sources and sinks on the diffusion process, is formulated as a nonlinear boundary value problem involving two coupled ordinary differential equations. An approximate analytic solution is presented and its validity is checked by finite differences. The qualitative effects of parameter changes are discussed.

INTRODUCTION

The CO₂ needed for photosynthesis in green plants is typically obtained by a diffusive flow along a pathway extending from the leaf exterior to the chloroplasts within the leaf. CO₂ diffuses from the ambient atmosphere through a boundary layer of relatively "still air" through open stomatal pores and into the substomatal cavity just inside the leaf. From there gaseous CO₂ diffuses through the intercellular air spaces (ias) to the cell walls of the mesophyll cells. Once the gaseous CO₂ has been absorbed into the cell wall liquid, it continues to diffuse as a solute through the plasmalemma membrane into the cell cytoplasm and finally into the chloroplasts where it is utilized in photosynthesis. CO₂ created by respiration within the cell (in the mitochondria) also diffuses into the chloroplasts.

Various models have been proposed to describe this phenomenon. An early paper by Brown and Escombe (1900) utilized an analogy from electrostatics. Their paper first introduced the resistance concept into plant physiology. It has become the standard model for quantitatively describing the CO₂ pathway.

The resistance model asserts that the steady state diffusive flux of CO₂ into the leaf, $J(\text{kg}/\text{m}^2\text{s})$, is proportional to the change in concentration (kg/m^3) between the atmosphere C^{atm} and the substomatal cavity C^{cav} :

$$J = (C^{\text{atm}} - C^{\text{cav}})/R^{\text{ent}} \quad [1]$$

where R^{ent} is the "entrance" resistance (s/m). The quantity R^{ent} depends upon the geometry of the stomatal pore, the thickness of the still air layer, and the diffusion coefficient. Since the time of the Brown and Escombe paper, many researchers have given expressions for R^{ent} . As an example of such an expression, we quote the result of Holcomb and Cooke (1977) and Cooke and Rand (1980):

Article was submitted for publication in June 1979; reviewed and approved for publication by the Soil and Water Division of ASAE in October 1979.

The authors are: R. H. RAND, Theoretical and Applied Mechanics Dept., and J. R. COOKE, Agricultural Engineering Dept., Cornell University, Ithaca, NY.

$$R^{\text{ent}} = (\mu/D)[T + \lambda\beta^2 / \alpha\beta^2 \ln(4/\alpha) - \beta] \quad [2]$$

where

- μ = semi-major axis of elliptical pore, cm
- D = diffusion coefficient of CO₂ in air, cm²/s
- T = ratio of boundary layer thickness to μ
- λ = ratio of pore depth to μ
- α = ratio of semi-minor to semi-major pore axes
- β = ratio of distance between neighboring stomata to μ .

While the resistance model of equation [1] gives J as a function of C^{atm} (measurable) and R^{ent} (calculable from equation [2]), it also requires that C^{cav} be known. Since C^{cav} is not easily measured, it is desirable to be able to calculate C^{cav} from additional theoretical considerations.

A typical approach to this question is given by the equation (Nobel, 1974)

$$J = \frac{C^{\text{cav}} - C^{\text{int}}}{R^{\text{int}}} \quad [3]$$

where C^{int} is taken to be a typical (solute) concentration of CO₂ in the chloroplasts and where R^{int} , not to be confused with R^{ent} , is the sum of resistances due to diffusion through the ias, cell wall, plasmalemma, cytoplasm, etc. Here each resistance in the series is taken to be of the form L/D where L is the length of the associated portion of the pathway and where D is the associated diffusion coefficient (equation [2]). (Nobel, 1974).

Although this procedure formally solves the problem of establishing a value for C^{cav} (equations [1] and [3]) represent two equations in the two unknowns J , C^{cav} , it involves certain theoretical objections which we will now discuss.

The process of CO₂ diffusion in the ias and in the mesophyll cells is fundamentally different from that in the entrance region. For example, while moving through the stomatal pore, CO₂ diffuses inward without being absorbed along the way. In the ias, however, CO₂ simultaneously diffuses inward and is absorbed into the mesophyll cell walls which bound the ias. It is a question of diffusion without distributed sinks and sources (in the entrance region) versus diffusion with distributed sinks and sources (in the ias and cell interiors).

The difference between these two processes can be exhibited by considering the following differential equation which is based on a simplified one-dimensional situation:

$$D \frac{d^2 C}{dx^2} = \Phi(C, x) \quad [4]$$

where the LHS (left hand side) represents diffusion and the RHS Φ represents distributed sinks (and sources). The special case $\Phi \equiv 0$ corresponds to the usual model of CO₂ diffusion without distributed sinks or sources, and has the solution:

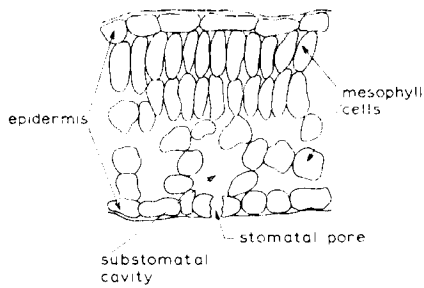


FIG. 1 Transverse section of a leaf (after Nobel, 1974, p. 3).

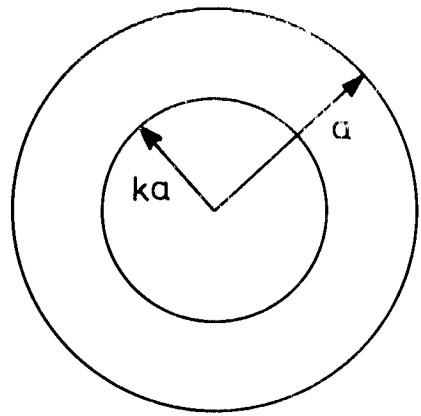


FIG. 2 An idealized spherical mesophyll cell. The region between the vacuole, $r = ka$, and the cell wall, $r = a$, contains distributed CO_2 sources and sinks.

$$C(x) = C(O) + [C(L) - C(O)](x/L) \dots\dots\dots [5]$$

and

$$J = -D \frac{dC}{dx} = -\frac{\Delta C}{R} \dots\dots\dots [6]$$

where $R = L/D$, where $C(O)$, $C(L)$ represent values of C at $x = 0, L$ and where $\Delta C = C(L) - C(O)$.

The case $\Phi \neq 0$ is, however, very different. The solution is unavailable for a general function $\Phi(C, x)$, although the equation may be solved in the case of particular choices for Φ . This equation has been used by Rand (1977, 1978) to model diffusive flow in the ias, and in a related three-dimensional form by Parkhurst (1977) to model leaf diffusion, and by Sinclair et al. (1977) and by Sinclair and Rand (1979) to model cellular diffusion.

Note that the expression for J in the case $\Phi \equiv 0$, equation [6], will generally not agree with the comparable expression when $\Phi \neq 0$. For example, if $\Phi \equiv \text{constant}$ then equation [4] has the solution

$$C(x) = (x^2 - Lx)(\Phi/2D) + C(O) + [C(L) - C(O)](x/L) \dots [7]$$

and

$$J = -D \frac{dC}{dx} = \left(\frac{L}{2} - x\right) \Phi - \frac{\Delta C}{R} \dots\dots\dots [8]$$

Note the extra term in equation [8] which is missing from equation [6].

Our purpose in the present paper is to use a relatively realistic model of the leaf CO_2 diffusion process which includes distributed sinks and sources in order to obtain an equation to supplement equation [1] (just as equation [3] does in the case where distributed sinks and sources are neglected). This new equation, together with equation [1], will describe the diffusion process.

We will derive an expression for J as a function of C^{cav} and the biochemical and geometrical parameters of the leaf. The complicated biochemistry of photosynthesis and respiration will be represented by Michaelis-Menten kinetics. Although many authors have used Michaelis-Menten kinetics to describe photosynthesis (Jones and Slatyer (1972) who give an extensive list of references), their models have usually omitted the effects of leaf geometry (i.e., cell size and cell distribution). These effects will be included in our treatment.

The resulting expression for J summarizes the process of CO_2 assimilation in leaves at a level of complexity appropriate for use in whole plant or crop simulation models.

THE MODEL

We shall be concerned with the diffusive flow of CO_2

from the substomatal cavity to the chloroplasts. Although this problem is perhaps most realistically modeled by using an accurate leaf geometry (Fig. 1), the boundary value problem which would result from such geometry would certainly be intractable: one would require the three dimensional diffusion equation to hold in the ias; an equation similar to equation [9] below, but without spherical symmetry, to hold in the mesophyll cell cytoplasm; and boundary conditions based on continuity of flux and Henry's law to hold at the liquid-gas interfaces. We shall present a model which basically includes these effects but in the context of a simplified geometry.

The model will involve gaseous diffusion in the ias and diffusion in the liquid phase in the mesophyll cells. We shall utilize two previous approaches which treated these problems separately; the ias model of Rand (1977, 1978) and the spherical mesophyll cell model of Sinclair et al. (1977) and of Sinclair and Rand (1979). The resulting model will provide a comprehensive analysis of CO_2 diffusion in the leaf. As will be apparent, the process of joining these two previously developed models together leads to a complicated mathematical problem (due to the appearance of coupling terms in the differential equations and boundary conditions) and is in no way simply a question of superimposing the previously obtained results. To deal with this coupled problem, we proceed as follows.

We first consider a single idealized spherical mesophyll cell (Fig. 2) (Sinclair et al., 1977; Sinclair and Rand, 1979). The region of cytoplasm contained between the vacuole ($r = ka$, $0 < k < 1$) and the cell boundary ($r = a$) is modeled as containing distributed sinks and sources of CO_2 , representing, respectively, photosynthesis and respiration. The variable $C^{cell}(r)$ which describes the CO_2 concentration in the cell at radius r is governed by the equation:

$$D_{cell} \nabla^2 C^{cell} = \Phi(C^{cell}) \dots\dots\dots [9]$$

where

$$\Phi = \Phi(C^{cell}) = \Phi_{chl} - \Phi_{pr} - \Phi_{drk} \dots\dots\dots [10]$$

- Φ_{chl} = chloroplast carboxylation rate, $\text{kg/m}^3\text{s}$
- Φ_{pr} = photorespiration rate, $\text{kg/m}^3\text{s}$
- Φ_{drk} = dark respiration rate, $\text{kg/m}^3\text{s}$

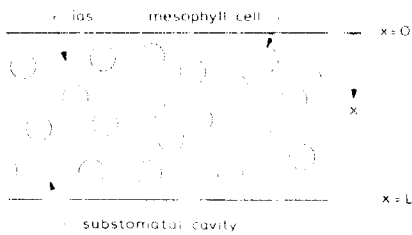


FIG. 3 Schematic diagram of the leaf model. The spherical mesophyll cells of Fig. 2 are actually assumed to be uniformly distributed throughout the intercellular air space (ias). The variable x measures distance in a direction perpendicular to the leaf surface.

$$\nabla^2 = 1/(r^2) d/(dr) (r^2 d/(dr)) \text{ for spherical symmetry}$$

D^{cell} = diffusion coefficient of CO_2 as a solute in cytoplasm.

Here the distributed sink term Φ is the algebraic sum of a photosynthetic sink term and two respiration source terms.

Following Sinclair et al. (1977) and Sinclair and Rand (1979) we will model Φ_{chl} and Φ_{pr} using Michaelis-Menten kinetics:

$$\Phi_{chl} = (V_c K_o C^{cell}) / (K_c K_o + K_o C^{cell} + K_c Q) \quad [11]$$

$$\Phi_{pr} = (t V_o K_c Q) / (K_c K_o + K_o C^{cell} + K_c Q) \quad [12]$$

where

- K = Michaelis-Menten constant, kg/m^3
- V = maximum enzymatic velocity, kg/m^3s
- Q = oxygen concentration, kg/m^3
- t = fraction of glycolate carbon released in photorespiration.

where subscripts c, o refer to CO_2 and oxygen respectively, and where Φ_{drk} has been taken as a constant.

Equation [9] is supplemented by the following boundary conditions:

At the vacuole,
 $r = ka, dC^{cell}/dr = 0, \text{ (no flux)}$ [13]

At the cell boundary,
 $r = a, C^{cell} = HC^{ias}, \text{ (Henry's law)}$ [14]

Henry's law, equation [14], provides the equilibrium condition at the gas-liquid interface. We apply it here to an idealized two component system of a dilute solution of CO_2 in water. The proportionality constant H is temperature dependent (Nobel, 1974, gives $H = 1.19$ at $10^\circ C$, $H = 0.88$ at $20^\circ C$). Henry's law has previously been applied to leaf diffusion field equations in Rand (1977, 1978).

We now consider the ias in which the spherical cells reside (Fig. 3). Rather than assume a particular configuration for the placement of cells (Rand, 1978), we will assume a uniform distribution which is characterized by the following two parameters:

Let

A^{mes}/A = surface area of mesophyll cells per leaf area A

V^{ias}/V = volume of ias per leaf volume V

where

A = area of leaf surface (one side of leaf only)

L = leaf thickness (Fig. 3)

V = AL = total leaf volume per leaf area A .

The parameters A^{mes}/A and V^{ias}/V have been extensively measured in real leaves (Turrell, 1936; Nobel, 1976; Nobel et al., 1975). They may be related to other parameters as follows:

Let

N = number of mesophyll cells under leaf area A

A^{ias} = effective cross-sectional area available for gaseous diffusion in the leaf interior, in a direction perpendicular to the leaf surface.

Then

$$N = A^{mes}/(4\pi a^2) \quad [15]$$

since $4\pi a^2$ is the surface area of a single spherical cell. Also

$$A^{ias}/A = V^{ias}/V \quad [16]$$

since the uniform distribution of cells requires that $V^{ias} = LA^{ias}$.

In order to derive an equation which describes $C^{ias}(x)$, the average concentration of CO_2 in the ias at cross-section x (Fig. 3), we consider a volume element Σ of thickness dx and of area A . For conservation of mass, the net rate at which CO_2 is added to Σ by gaseous diffusion from the rest of the ias must equal the rate at which CO_2 is absorbed into the mesophyll cells in Σ (at steady state):

$$\left(\frac{dJ^{ias}}{dx} dx \right) A^{ias} = J^{cell} A^{mes} \left(\frac{dx}{L} \right) \quad [17]$$

where

$$J^{ias} = -D^{ias} (dC^{ias}/dx) \quad [18]$$

$$J^{cell} = -D^{cell} (dC^{cell}/dr) \Big|_{r=a} \quad [19]$$

That is,

$$\frac{d^2 C^{ias}}{dx^2} = \left(\frac{D^{cell}}{D^{ias}} \right) \left(\frac{A^{mes}}{A^{ias}} \right) \left(\frac{1}{L} \right) \frac{dC^{cell}}{dr} \Big|_{r=a} \quad [20]$$

Equation [20] is accompanied by the following boundary conditions:

At the leaf interior,

$$x = 0, dC^{ias}/dx = 0 \text{ (no flux)} \quad [21]$$

At the substomatal cavity,

$$x = L, C^{ias} = C^{cav} \text{ (continuity)} \quad [22]$$

Note that equations [20]-[22] for $C^{ias}(x)$ and equations [9]-[14] for $C^{cell}(r)$ are coupled (specifically through the appearance of dC^{cell}/dr in equation [20] and of C^{ias} in equation [14].)

If these equations could be solved simultaneously we would have $C^{ias}(x)$ and $C^{cell}(r)$ as functions of C^{cav} (equation [22]). Then the problem would be completed by requiring conservation of mass for the CO_2 flow into the leaf:

$$J_A = D^{ias} (dC^{ias}/dx) \Big|_{x=L} A^{ias} \quad [23]$$

Here equation [23] would provide the desired expression relating J to C^{cav} (since $C^{ias}(x)$ depends on C^{cav}), which would replace equation [3] in supplementing equation [1]. In summary, equation [23] could be solved simultaneously with equation [1] to eliminate C^{cav} from the problem and to thereby obtain an expression for J as a function of the biochemical and geometrical model parameters.

AN APPROXIMATE FORMULA

The equations [9]-[14] and [20]-[22] are complicated mathematically and their analytical solution is unavailable. In view of this mathematical difficulty we shall presently derive an approximate formula for J which is based on certain simplifying assumptions. In the next section of this paper we discuss the validity of this formula and show that it does in fact follow as an acceptable approximation from the differential equation model just presented.

In deriving the following approximate formula we shall neglect the variation in CO_2 concentration from point to point within the leaf interior. In fact this concentration will drop as CO_2 diffuses further inward and is assimilated. Nevertheless if the maximum CO_2 concentration drop is small compared to C^{cav} , then the assumption of constant concentration will introduce only a small error.

As in boundary condition [14], we assume Henry's law governs the equilibrium of gaseous CO_2 with the CO_2 dissolved in the cell liquid:

$$C^{cell} = H C^{ias} \quad [24]$$

Neglecting any drops in CO_2 concentration due to diffusion, we assume that all the CO_2 in the liquid phase is at the same concentration C^{cell} , and likewise that all the CO_2 in the gaseous phase is at the same concentration C^{ias} . In particular this means that C^{ias} equals C^{cav} so that equation [24] becomes

$$C^{cell} = H C^{cav} \quad [25]$$

From equations [10], [25] the assimilation rate per unit volume inside a mesophyll cell is assumed to be independent of position and equals $\Phi(HC^{cav})$. (Here the notation $\Phi(HC^{cav})$ means replace C^{cell} by HC^{cav} whenever it appears in equations [10]-[12]). The assimilation rate of one cell becomes

$$(4\pi/3)(a^3 - k^3 a^3) \Phi(HC^{cav}) \quad [26]$$

where the first factors represent the volume of the portion of the cell which lies in the region $ka < r < a$ (Fig. 2).

The flux J into the mesophyll cells under a leaf area A equals N times expression [26]. Using equation [15], we obtain

$$J = \frac{A^{mes} a(1-k^2)}{A \cdot 3} \Phi(HC^{cav}) \quad [27]$$

Equation [27] is an approximate algebraic formula for J in terms of C^{cav} . By simultaneously solving equations [27] and [1], C^{cav} can be eliminated, yielding an expression for J . This involves solving only a quadratic equation. In a later section of this paper we will discuss the resulting expression for J . Before doing so, however, we shall first relate equation [27] to the differential equation

model formulated in the previous section. We shall also justify the severe assumptions made in the derivation of equation [27] (namely that drops in CO_2 concentration are negligible).

VALIDITY OF THE APPROXIMATE FORMULA

In this section we will show analytically that equations [9]-[23] exhibit formula [27] as an approximate solution. We will also show by numerical integration of the differential equations that the approximation is valid for typical values of the model parameters.

We begin by nondimensionalizing the model equations [9]-[14], [20]-[23]. We replace the variables C^{cell} , C^{ias} , r and x by the nondimensional variables:

$$\begin{aligned} u &= C^{cell}/K_c \\ v &= C^{ias}/K_c \\ \rho &= r/a \\ \xi &= x/L \end{aligned} \quad [28]$$

Equation [9] becomes

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{du}{d\rho} \right) = F(u) \quad [29]$$

where

$$F(u) = \sigma \left(\frac{u-\Gamma}{u+\gamma} \right) \quad [29.1]$$

$$\sigma = (a^2 V_c / D^{cell} K_c) (1 - \Phi_{drk} / V_c) \quad [29.2]$$

$$\gamma = 1 + Q/K_o \quad [29.3]$$

$$\Gamma = \frac{t(V_o/V_c)(Q/K_o) + (\Phi_{drk}/V_c)(1+Q/K_o)}{1 - \Phi_{drk}/V_c} \quad [29.4]$$

(Here Γ is a dimensionless compensation concentration. Nobel (1974), p. 338).

The boundary conditions [13], [14], become

$$\rho = k, du/d\rho = 0 \quad [30]$$

$$\rho = 1, u = Hv \quad [31]$$

Equation [20] becomes

$$\frac{d^2 v}{d\xi^2} = G(v) \quad [32]$$

where

$$G(v) = \Lambda (du/d\rho) \Big|_{\rho=1} \quad [32.1]$$

$$\Lambda = (D^{cell}/D^{ias})(A^{mes}/A)(V/V^{ias})(L/a) \quad [32.2]$$

The boundary conditions [21], [22] become

$$\xi = 0, dv/d\xi = 0 \quad [33]$$

$$\xi = 1, v = v^{cav} \quad [34]$$

Equation [23] becomes

$$J = D^{ias} (v^{ias}/V)(K_c/L)(dv/d\xi) \Big|_{\xi=1} \quad [35]$$

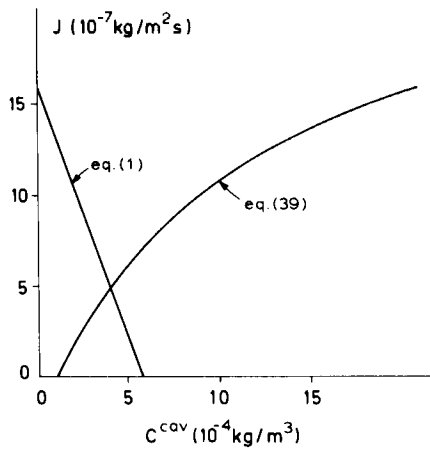


FIG. 4 Graphs of equations [1] and [39] for parameter values of equations [38]. The graph of equation [39] has a horizontal asymptote at $J = 26.3 \times 10 \text{ kg/m}^2\text{s}$.

In the Appendix we obtain an approximate solution to equations [29]-[31] by expanding $F(u)$ in a power series about $u = Hv$ and neglecting terms of order $(u-Hv)^2$. This assumes that the variation in CO_2 concentration u throughout the cytoplasm of a cell is small. We also assume a certain parameter ω is small (see Appendix for details). The resulting approximate solution $(u(p))$ may be differentiated to give the RHS of equation [32]:

$$G(v) = (\Lambda/3)(1-k^3)F(Hv) \dots\dots\dots [36]$$

Also in the Appendix we obtain an approximate solution to equations [32]-[34], with $G(v)$ as in equation [36]. We expand $G(v)$ in a power series about $v = v^{cav}$ and neglect terms of order $(v-v^{cav})^2$. This assumes that the variation in CO_2 concentration v throughout the ias of the leaf is small. We also assume a certain parameter Ω is small (see Appendix for details). The resulting approximate solution $v(\xi)$ may be differentiated to give the RHS of equation [35]:

$$(dv/d\xi)|_{\xi=1} = (\Lambda/3)(1-k^3)F(Hv^{cav}) \dots\dots\dots [37]$$

Substituting this result into equation [35] and using equations [29.1], [32.2] we obtain the approximate formula [27].

Thus we have shown that the approximate formula of the previous section is an approximate solution of the differential equation model. How good is this approximation? We have assumed in the derivation that various drops in concentration and certain parameters were small. In order to test the validity of these assumptions, we numerically integrated equations [29]-[34] in the following way: First we wrote equations [29] and [32] in finite difference form using central differences. Then we numerically solved equations [29]-[31] by using the boundary condition [30] and selecting the value of u at $p = k$ arbitrarily. In particular we computed u and du/dp at $p = 1$. By repeating this process for different values of u at $p = k$ we were able to numerically construct the function $G(v)$ (which relates du/dp at $p = 1$ to $u = Hv$ at $p = 1$).

Next we numerically solved equations [32]-[34], interpolating the required values for $G(v)$ (which appears in the RHS of equation [32]) from those obtained by

numerically integrating equation [29]. We used the boundary condition [33] and selected the value of v at $\xi = 0$ arbitrarily. By repeating this process for different values of v at $\xi = 0$ we were able to numerically calculate corresponding values of v and $dv/d\xi$ at $\xi = 1$. Then using equations [34] and [35] we obtained values of J as a function of C^{cav} (which equals $v^{cav}K_c$).

By solving this latter relationship simultaneously with equation [1] we eliminated C^{cav} and were able to find J for a given set of the model parameters.

For example, we used the following values of the geometrical and biochemical parameters (most of these are taken from Sinclair et al. (1977), where references are given to the experimental literature; also see Cooke and Rand (1980) for parameter values):

- $Q/K_o = 0.7$
- $\Phi_{drk}/V_c = 0.03$
- $t = 0.25$
- $V_o/V_c = 0.5$
- $V_c = 0.2 \text{ kg/m}^3\text{s}$
- $K_c = 7 \times 10^{-4} \text{ kg/m}^3$
- $a = 5 \times 10^{-6} \text{ m}$
- $D^{cell} = 1.8 \times 10^{-9} \text{ m}^2/\text{s}$
- $D^{ias} = 1.6 \times 10^{-5} \text{ m}^2/\text{s}$
- $A^{mes}/A = 30$
- $v^{ias}/V = 0.35$
- $L = 250 \times 10^{-6} \text{ m}$
- $H = 1$
- $k = 0.9$
- $R^{ent} = 3.7 \times 10^2 \text{ s/m}$
- $C^{atm} = 5.88 \times 10^{-4} \text{ kg/m}^3 \dots\dots\dots [38]$

With these parameter values the numerical integration procedure gave $J = 4.93 \times 10^{-7} \text{ kg/m}^2\text{s}$. Substituting these same parameter values into equations [27] and [1] we find $J = 5.00 \times 10^{-7} \text{ kg/m}^2\text{s}$. Thus for the typical parameters of equations [38] the approximate formula checks with the numerical integration of the model equations to within 2 percent.

DISCUSSION

We return to a discussion of the approximate formula [27], which may be written (using equations [10]-[12]):

$$J = \frac{A^{mes}}{A} \frac{a(1-k^3)}{3} V_c \left\{ \frac{HC^{cav} - t \frac{V_o}{V_c} \frac{Q}{K_o}}{HC^{cav} + 1 + \frac{Q}{K_o}} - \frac{\Phi_{drk}}{V_c} \right\} \dots\dots\dots [39]$$

This equation is to be solved simultaneously with equation [1] which is rewritten here for convenience:

$$J = \frac{C^{atm} - C^{cav}}{R^{ent}} \dots\dots\dots [1]$$

By equating the RHS's of equations [39] and [1] we obtain quadratic equation on C^{cav} . One of its roots is

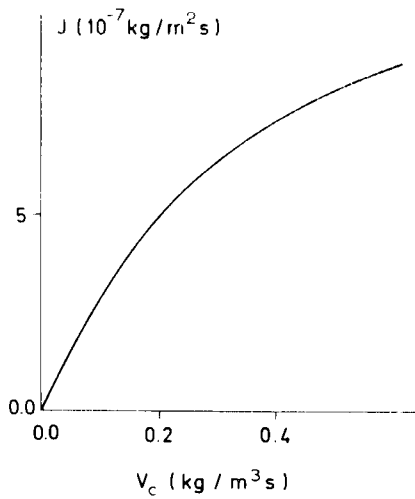


FIG. 5 J shown as a function of V_c according to the approximate equation [39] and equation [1]. Values of the other parameters are as in equations [38].

negative and must be rejected as extraneous. The other root is positive and the resulting value of C^{cav} may be found in a straightforward manner by use of the quadratic formula. Once C^{cav} is known, J may be found immediately from equation [1].

For a particular problem with a fixed set of model parameters the algebraic procedure just described is the best and most direct way of finding J. To discuss general trends, however, we shall find it useful to consider a geometrical approach. By plotting equations [39] and [1] with respect to J and C^{cav} axes, we may identify their common solution as the point of intersection of their graphs.

The graph of equation [39] in the J- C^{cav} plane is a "saturation" curve (Fig. 4). It intersects the C^{cav} axis at $C^{cav} = K_c \Gamma / H$ where Γ is the dimensionless compensation concentration of equation [29.4]. This graph has a horizontal asymptote at

$$J = \frac{A^{mes}}{A} \frac{a(1-k^3)}{3} (V_c - \Phi_{drk}) \dots\dots\dots [40]$$

The graph of equation [1] is a straight line with slope $1/R^{ent}$. Its C^{cav} -axis intercept is C^{atm} while its J-axis intercept is C^{atm}/R^{ent} (Fig. 4).

The effect on J of changing a particular parameter may be stated in terms of the effect on the graphs of equations [39], [1]. E.g. it is clear from Fig. 4 that increasing R^{ent} decreases the slope of equation [1], and decreases J. Similarly increasing C^{atm} moves the straight line of Fig. 4 away from the origin (its slope remaining fixed), which causes an increase in J.

The effect of changing the other model parameters on the graph of equation [39] may be similarly investigated. If the C^{cav} intercept of equation [39] remains fixed, an increase in the horizontal asymptote of equation [39] as given by equation [40] will cause an increase in J. In this way we may conclude that increases in A^{mes}/A and in cell radius a cause increases in J, while an increase in vacuole size k decreases J. Similarly if the horizontal asymptote given by equation [40] remains fixed but the C^{cav} intercept decreases, then J increases. Now since the C^{cav} intercept is $K_c \Gamma / H$ we may conclude from equation [29.4]

that J increases with increases in H and K_c while J decreases with increases in K_c , t, V_c and Q. In a similar way we may determine that J increases with an increase in V_c but decreases with an increase in Φ_{drk} (although changes in these parameters cause both the C^{cav} intercept and the horizontal asymptote to change).

These effects may be summarized as follows:

$$J \uparrow \text{ with } \uparrow \text{ in: } C^{atm}, A^{mes}/A, a, H, K_c, V_c$$

$$J \downarrow \text{ with } \uparrow \text{ in: } R^{ent}, k, K_c, t, V_c, Q, \Phi_{drk} \dots\dots\dots [41]$$

Up to now we have taken the point of view that if the model parameters are given then we may use the approximate formula [39] to find J. On the other hand, if J is known from experimental measurements then equation [39] may be used to infer a value for one of the other model parameters.

Of the various model parameters used in equation [38], the one which is least reliably known is V_c . (For example, Sinclair et al., 1977, refer to values of V_c based on *in vitro* measurements, but they state that "*in vitro* determinations of V_c are almost certainly too small compared with *in vivo* determinations"). In order to find J as a function of V_c (for values of the other model parameters as in equation [38]) we may use the algebraic approach referred to above (this entails solving a quadratic equation based on equations [39], [1].) The result is shown in Fig. 5. We find that for $J = 5 \times 10^{-7} \text{ kg/m}^2 \text{ s}$ (a typical value; Nobel, 1974; Cooke and Rand, 1980), $V_c = 0.2 \text{ kg/m}^3 \text{ s}$. This value is about seven times larger than the *in vitro* determinations of V_c quoted in Sinclair et al. (1977) (although our other biochemical parameters agree with those in their paper). Our point is not to insist upon one value of V_c or another, but rather to show how the approximate formula [39] may be used to predict model parameters if J is known.

SUMMARY AND CONCLUSIONS

We have derived an approximate formula which governs CO_2 assimilation in leaves. It is based on a comprehensive model which emphasizes both geometry and Michaelis-Menten biochemistry, and which includes the effects of sources and sinks on the diffusion process.

The approximate formula has been shown to be an approximate solution to the differential equations of the model. The approximation has been verified by numerical integration of the model equations.

The qualitative effects of parameter changes on the CO_2 flux J have been discussed and are summarized in expression [41].

We feel that this formulation offers the most accurate expression currently available for J in terms of basic leaf parameters. It provides a substantial improvement over the usual method of predicting J (which is based on estimating a value for R^{int} (cf. equation [13]) in the context of a diffusion model which omits the effects of sources and sinks).

The approximate formula is sufficiently compact to be usable in a crop simulation model of the entire crop system.

References

1 Brown, H. T. and F. Escombe. 1900. Static diffusion of gases and liquids in relation to the assimilation of carbon and translocation in plants. Philos. Trans. Roy. Soc. B 193, 223.

2 Cooke, J. R. and R. H. Rand. 1980. Diffusion resistance models, in predicting photosynthesis for ecosystem models. eds. J. D. Hesketh and J. W. Jones, CRC Press Vol. I, Chap. 5.

3 Holcomb, D. P. and J. R. Cooke. 1977. An electrolytic tank analog determination of stomatal diffusion resistance. ASAE Paper No. 77-5510. ASAE, St. Joseph, MI 49085.

4 Jones, H. G. and R. O. Slatyer. 1972. Estimation of the transport and carboxylation components of the intracellular limitation to leaf photosynthesis. *Plant Physiology* (50):283.

5 Nobel, P. S. 1974. Intro. to biophysical plant physiology. Freeman.

6 Nobel, P. S. 1976. Photosynthetic rates of sun versus shade leaves of *Hyptis emoryi* Torr. *Plant Physiology* (58):218.

7 Nobel, P. S., L. J. Zaragoza and W. K. Smith. 1975. Relation between mesophyll surface area, photosynthetic rate, and illumination level during development for leaves for *Plectranthus parviflorus* Henckel. *Plant Physiology* (55):1067.

8 Parkhurst, D. F. 1977. A three-dimensional model for CO₂ uptake by continuously distributed mesophyll in leaves. *J. Theor. Biol.* (67):471.

9 Rand, R. H. 1977. Gaseous diffusion in the leaf interior. *TRANSACTIONS of the ASAE* 20(4):701.

10 Rand, R. H. 1978. A theoretical analysis of CO₂ absorption in sun versus shade leaves, *J. Biomechanical Engr., Trans. ASME* (100):20.

11 Sinclair, T. R., J. Goudriaan and C. T. deWit. 1977. Mesophyll resistance and CO₂ compensation concentration in leaf photosynthesis models. *Photosynthetica* (11):56.

12 Sinclair, T. R. and R. H. Rand. 1979. Mathematical analysis of CO₂ assimilation under high CO₂ concentrations. *Photosynthetica* (13):239.

13 Turrell, F. M. 1936. The area of the internal exposed surface of dicotyledon leaves. *Am. J. Bot.* (23):255.

APPENDIX

In this appendix we provide the mathematical details of the derivation of the approximate solution of equations [29]-[35] referred to in the text.

Expanding F(u) of equation [29.1] in a power series about u = Hv,

$$F(u) = F(Hv) + F'(Hv)(u-Hv) + \dots \quad [A1]$$

Neglecting higher order terms in equation [A1], equation [29] becomes

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{du}{d\rho} \right) = A_1 + A_2 u \quad [A2]$$

where

$$A_1 = F(Hv) - HvF'(Hv) \\ = \frac{\sigma(H^2 v^2 - 2\Gamma Hv - \Gamma\gamma)}{(Hv + \gamma)^2} \quad [A2.1]$$

$$A_2 = F'(Hv) \\ = \frac{\sigma(\gamma + \Gamma)}{(Hv + \gamma)^2} \quad [A2.2]$$

Equations [A2], [30], [31] have the solution

$$u = -\frac{A_1}{A_2} + \frac{1}{\rho} \left(Hv + \frac{A_1}{A_2} \right) \left(\frac{\cosh \omega \rho + M \sinh \omega \rho}{\cosh \omega + M \sinh \omega} \right) \quad [A3]$$

where

$$M = (1 - \omega k \tanh \omega k) / (\omega k - \tanh \omega k)$$

$$\omega = \sqrt{A_2}$$

Equation [A3] yields

$$\left. \frac{du}{d\rho} \right|_{\rho=1} = \left(Hv + \frac{A_1}{A_2} \right) \left[\frac{\omega(1-k) + (\omega^2 k - 1) \tanh \omega(1-k)}{\omega k + \tanh \omega(1-k)} \right] \quad [A4]$$

Expanding tanh ω(1-k) in a Maclaurin series,

$$\tanh \omega(1-k) = \omega(1-k) - \frac{\omega^3(1-k)^3}{3} + \dots \quad [A4.1]$$

Neglecting higher order terms in equation [A4.1] and substituting into equation [A4] gives

$$\left. \frac{du}{d\rho} \right|_{\rho=1} = \frac{(1-k^3)}{3} (Hv A_2 + A_1) \quad [A5]$$

Equation [A5] together with equations [A2.1], [A2.2], [32.2] give the expression for G(v) of equation [36].

Expanding G(v) of equation [36] in a power series about v = v^{cav},

$$G(v) = G(v^{cav}) + G'(v^{cav})(v - v^{cav}) + \dots \quad [A6]$$

Neglecting higher order terms in equation [A6], equation [32] becomes

$$\frac{d^2 v}{d\xi^2} = B_1 + B_2 v \quad [A7]$$

where

$$B_1 = G(v^{cav}) - v^{cav} G'(v^{cav}) \\ = \frac{\Lambda \sigma(1-k^3) (H^2 v^{cav2} - 2\Gamma Hv^{cav} - \Gamma\gamma)}{3(Hv^{cav} + \gamma)^2} \quad [A7.1]$$

$$B_2 = G'(v^{cav}) \\ = \frac{\Lambda \sigma H(1-k^3)(\gamma + \Gamma)}{3(Hv^{cav} + \gamma)^2} \quad [A7.2]$$

Equations [A7], [33], [34] have the solution

$$v = -\frac{B_1}{B_2} + \left(v^{cav} + \frac{B_1}{B_2} \right) \frac{\cosh \Omega \xi}{\cosh \Omega} \quad [A8]$$

where

$$\Omega = \sqrt{B_2}$$

$$\left. \frac{dv}{d\xi} \right|_{\xi=1} = \left(v^{cav} + \frac{B_1}{B_2} \right) \Omega \tanh \Omega \quad [A9]$$

Expanding tanh Ω in a Maclaurin series,

$$\tanh \Omega = \Omega - \dots \quad [A9.1]$$

Neglecting higher order terms in equation [A9.1] and substituting into equation [A9] gives

$$\left. \frac{dv}{d\xi} \right|_{\xi=1} = \frac{\Lambda(1-k^3)}{3} \frac{\sigma(Hv^{cav} - \Gamma)}{(Hv^{cav} + \gamma)} \quad [A10]$$

which together with equation [29.1] gives equation [37].